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(54) Modified MEK1 and MEK2, crystal of a peptide: ligand: cofactor complex containing such modified MEK1 or MEK2, and methods of use thereof

(57) Modified MEK1 peptides and modified MEK2 peptides, polynucleotides encoding those peptides, and methods for purifying the peptides and crystallizing them as peptide: cofactor: ligand complexes have been discovered. The three-dimensional structures of MEK1 peptide and MEK2 peptide, including the cofactor-and ligand-binding pockets, and uses of this information, for example, in molecular replacement and the modification, design and screening of compounds that may associate with MEK1, MEK2, or peptides structurally related thereto, have also been discovered.

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Description

FIELD OF THE INVENTION

[0001] The present invention generally relates to forms of a MEK1 peptide and forms of MEK2 peptide, crystals of a MEK1 or MEK2 peptide : ligand : cofactor complex, methods for producing those crystals, three-dimensional structural information derived from crystallographic data and to methods using that structural information.

BACKGROUND OF THE INVENTION

[0002] Mitogen-activated protein (MAP) kinases are thought to act as an integration point for multiple biochemical signals because they are activated by a wide variety of extracellular signals. The pattern of MAP kinase (MAPK) cascade is not restricted to growth factor signaling and it is now known that signaling pathways initiated by phorbol esters, ionophors, heat shock, and ligands for seven transmembrane receptors use distinct MAP kinase cascades with little or no cross-reactivity between them.

[0003] Multiple MAP kinases have been described in yeast including SMK1, HOG1, MPK1, FUS3, and KSS1. In mammals, the MAP kinases have been identified as extracellular signal-regulated kinase (ERK), c-Jun amino-terminal kinase (JNK), and p38 kinase (Davis, *Trends Biochem. Sci.* 19: 470 (1994)). These highly conserved MAP kinase isoforms are activated by dual phosphorylation on threonine and tyrosine residues.

[0004] A critical protein kinase lies upstream of the MAP kinase-mediated signaling pathway and stimulates the enzymatic activity of MAP kinases. The structure of this protein kinase, denoted MEK1, for MAP kinase /ERK kinase, was elucidated from a complementary DNA sequence and shown to be a protein of 393 amino acids (43.5-kD) that is related most closely in size and sequence to the product encoded by the *Schizosaccharomyces pombe* byr1 gene (Crews *et al.*, *Science* 258: 478-480 (1992)). The MEK gene was highly expressed in murine brain, and the product expressed in bacteria phosphorylated the ERK gene product *in vitro.* As an essential component of the MAP kinase signal transduction pathway, MEK1 is involved in many cellular processes such as proliferation, differentiation, transcription regulation and development.

[0005] A cDNA encoding the human homolog of MEK1 was cloned from a human T-cell cDNA library, GenBank Accession Number L11284 (Seger *et al. J. Biol. Chem.*267: 25628-25631 (1992)). When overexpressed in COS cells, the predicted 43,439-Da protein led to increased phorbol ester-stimulated MAP kinase kinase activity. The human MEK1 shares 99% amino acid sequence identity with the murine MEK1 and 80% with human MEK2. Human MEK1 and MEK2 encode 393 and 400 amino acid residues, respectively. Both MEK1 and MEK2 were expressed in *E. coli* and shown to be able to activate recombinant human ERK1 *in vitro.* The purified MEK2 peptide stimulated threonine and tyrosine phosphorylation on ERK1 and concomitantly activated ERK1 kinase activity more than 100-fold. The recombinant MEK2 showed lower activity as an ERK activator as compared with MEK2 purified from tissue. However, the recombinant MEK2 can be activated by serum-stimulated cell extract *in vitro.* MEKs, in a manner similar to ERKs, are likely to consist of a family of related proteins playing critical roles in signal transduction. (Zheng *et al., J. Biol. Chem.* May 25; 268(15): 11435-9 (1993))

[0006] Constitutive activation of MEK1 results in cellular transformation. This protein kinase therefore represents a likely target for pharmacological intervention in proliferative and inflammatory diseases (Lee *et al.*, *Nature* 372, 739-746 (1994); Dudley *et al., Proc. Natl. Acad. Sci. U.S.A.* 92, 7686-7689 (1995)). In order to identify small-molecule inhibitors of this pathway, Sebolt-Leopold *et al.* developed an *in vitro* cascade assay using recombinantly expressed glutathione-S-transferase fusion proteins of MEK1 and ERK1 (Sebolt-Leopold *et al., Nature Med.* 5: 810-816(1999)). Sebolt-Leopold *et al.* also reported the discovery of a highly potent and selective inhibitor of MEK1, 2-(2-chloro-4-iodo-phenylamino)-N-cyclopropylmethoxy-3,4-difluoro-benzamide. This article reported that after treatment with this inhibitor, tumor growth was inhibited as much as 80% in mice with colon carcinomas of both mouse and human origin. Efficacy was achieved with a wide range of doses with no signs of toxicity, and correlated with a reduction in levels of MAPK in excised tumors. It was concluded that these data indicate that MEK inhibitors represent a promising, non-cytotoxic approach to the clinical management of colon cancer.

[0007] Influenza A viruses are significant causes of morbidity and mortality worldwide. Annually updated vaccines may prevent disease, and anti-virals are effective treatment early in disease when symptoms are often nonspecific. Viral replication is supported by intracellular signaling events. Using a nontoxic inhibitor of MEK1 and MEK2, and thus an inhibitor of the RAF1/MEK/ERK pathway, Pleschka *et al.* examined the cellular response to infection with influenza A. The inhibitor suppressed both the early and late ERK activation phases after virus infection. Inhibition of the signaling pathway occurred without impairing the synthesis of viral RNA or protein, or the import of viral ribonucleoprotein complexes (RNP) into the nucleus (Pleschka *et al., Nature Cell Biol.* 3: 301-305 (2001)). Instead, it inhibited RAF/MEK/ERK signaling and the export of viral RNP without affecting the cellular mRNA export pathway. It was proposed that ERK regulates a cellular factor involved in the viral nuclear export protein function. An experiment using a nontoxic

inhibitor of MEK1 and MEK2 to examine the cellular response to infection with influenza A suggested that local application of MEK inhibitors may have only minor toxic effects on the host while inhibiting viral replication without giving rise to drug-resistant virus variants (Pleschka *et al., Nature Cell Biol.* 3: 301-305 (2001)).

[0008] Ryan *et al.* showed that inhibition of MEK1 blocks p53-induced NF-kappa-B activation and apoptosis but not cell-cycle arrest. They demonstrated that p53 activates NF-kappa-B through the RAF/MEK1/p90(rsk) pathway rather than the TNFR1/TRAF2/IKK pathway used by TNFA *(Nature* 404: 892-897 (2000)).

[0009] One such means of mediating signal transduction through the MEK1 pathway is to identify enhancers or inhibitors to the MEK1 peptide. Such identification has heretofore relied on serendipity and/or systematic screening of large numbers of natural and synthetic compounds. A superior method of drug development relies on structure assisted drug design. In this case, the three-dimensional structure of a peptide-inhibitor complex is determined and potential enhancers and/or potential inhibitors are screened and/or designed with the aid of computer modeling [Bugg *et al.*, Scientific American, Dec.: 92-98 (1993); West *et al.*, TIPS, 16: 67-74 (1995); Dunbrack *et al.*, Folding & Design, 2: 27-42 (1997)]. However, heretofore the three-dimensional structure of the MEK1 peptide or MEK2 peptide has remained unknown, essentially because no MEK1 peptide or MEK2 peptide crystals have been produced of sufficient quality to allow the required X-ray crystallographic data to be obtained. Therefore, there is presently a need for obtaining a form of the MEK1 peptide or MEK2 peptide that can be crystallized with a ligand (such as an inhibitor) to form a crystal with sufficient quality to allow such crystallographic data to be obtained. Further, there is a need for such crystals. There is also a need for the determination of the three-dimensional structure of such crystals. Finally, there is a need for procedures for related structural based drug design and/or screening based on the crystallographic data.

[0010] USP 5,663,314 to Seger *et al.* discloses two types of MEK1 peptides, namely, MKK1a and MKK1b and nucleotide encoding them. MKK1a has 399 amino acid residues and MKK1b has 368 amino acid residues that is identical to MKK1a except lacking amino acid residues from 147 to 172. The modification of the MEK1 peptide by truncation of the NH_2-terminal region or by removal or replacement of the insertion loop-forming region, or by a combination of these modifications to improve the peptide's biophysical characteristics, especially with respect to crystallizability, has not previously been reported.

[0011] The citation of any reference herein should not be construed as an admission that such reference is available as "Prior Art" to the instant application.

SUMMARY OF THE INVENTION

[0012] The present invention provides modified MEK1 peptide and modified MEK2 peptide amino acid sequences, and methods for producing such modified MEK1 and MEK2 peptide sequences. In one embodiment, the MEK1 and MEK2 peptides may be modified omitting a significant portion of the NH_2-terminal region of the MEK1 and MEK2 peptides (hereinafter referred to as "NH_2-terminally truncated MEK1 peptide" and "NH_2-terminally truncated MEK2 peptide", respectively, or collectively as "NH_2-terminally truncated MEK1 and MEK2 peptides") and/or by deletion of the MEK1 insertion loop domain and/or by replacement of the MEK1 insertion loop domain with a linker peptide (hereinafter, MEK1 or MEK2 having either one or all of these modifications is referred to as "modified MEK1," "modified MEK2," or collectively as "modified MEK1 and MEK2").

[0013] The NH_2-terminally truncated MEK1 peptides lack at least 30 amino acid residues from the NH_2-terminal region of the full-length peptide. Preferably, the NH_2-terminally truncated MEK1 peptides lack at least 30 to at most 70 amino acid residues, more preferably 41 to 61 amino acid residues from the NH_2-terminal region of the full-length peptide, or a conservatively substituted variant thereof.

[0014] The NH_2-terminally truncated MEK2 peptides lack at least 34 amino acid residues from the NH_2-terminal region of the full-length peptide of SEQ ID NO: 4. Preferably, the NH_2-terminally truncated MEK2 peptides lack at least 34 to at most 74 amino acid residues, more preferably 45 to 65 amino acid residues from the NH_2-terminal region of the full-length peptide, or a conservatively substituted variant thereof.

[0015] In another embodiment, the modified MEK1 peptide may have a deletion of insertion loop-forming amino acid residues, particularly from amino acid 280 to amino acid 323 of SEQ ID NO: 2; or at least 40 amino acids from between amino acid residue 264 and amino acid 310 of SEQ ID NO: 2. This may include a deletion of amino acids (1) from amino acid 264 to amino acid 310 of SEQ ID NO: 2; (2) from amino acid 270 to amino acid 310 of SEQ ID NO: 2; (3) from amino acid 264 to amino acid 305 of SEQ ID NO: 2; (4) amino acid 267 to amino acid 307 of SEQ ID NO: 2; or (5) from amino acid 265 to amino acid 304 of SEQ ID NO: 2.

[0016] Alternatively, the MEK1 insertion loop domain may be replaced by with a linker peptide, wherein the linker peptide may have at most 10 amino acid residues. Preferably, the linker peptide has the amino acid sequence of Lys-Asn-Cys-Lys-Thr-Asp.

[0017] The modified MEK1 peptides of the invention may be modified by any one or any combination of the NH_2-terminal truncation, the deletion of insertion loop-forming amino acid residues, and the replacement of the MEK1 insertion loop domain with a linker peptide described above.

[0018] The invention further provides peptides that are defined by the three-dimensional structural coordinates of the MEK1 or MEK2 peptides as set forth in Table 1 or Table 2 respectively, or of related peptides which possess the structural coordinates having a root mean square deviation of not more than about 1.25 Å away from the core C alpha atoms of the MEK1 or MEK2 peptides as set forth in Table 1 or Table 2.

[0019] Additionally, the invention provides peptides that comprise a MEK1, MEK2 or MEK-like cofactor or ligand binding pocket, as defined below.

[0020] The invention further provides isolated, purified polynucleotides, which encode the modified MEK1 and/or MEK2 peptide sequences. The polynucleotides may be natural or recombinant.

[0021] The invention further provides expression vectors for producing the modified MEK1 and MEK2 peptides in a host cell. It further provides host cells which may be stably transformed and transfected with a polynucleotide encoding the modified MEK1 peptides or modified MEK2 peptides, or a fragment thereof or an analog thereof, in a manner allowing the expression of the modified MEK1 peptides or MEK2 peptides. The present invention additionally includes cells transfected or transformed with an expression vector of the present invention. The present invention also includes methods for expressing a modified MEK1 peptide or modified MEK2 peptide comprising culturing a cell that expresses the modified MEK1 peptide or modified MEK2 peptide in an appropriate cell culture medium under conditions that provide for expression of the peptide by the cell.

[0022] Methods of purifying the modified MEK1 peptides or modified MEK2 peptides of the invention from a fermentation broth containing the modified MEK1 peptide or modified MEK2 peptide, respectively, and contaminant proteins other than the MEK1 peptide or MEK2 peptide, respectively, is also provided. The methods comprise subjecting the fermentation broth to immobilized metal chelate chromatography, which may preferably comprise pyrrole-2-carboxylate and/or zinc.

[0023] The invention also provides methods of using the purified modified MEK1 peptide or mofidied MEK2 peptide to produce ternary complexes of peptide: ligand: cofactor, and for producing crystals of the peptide: ligand: cofactor complexes containing the modified MEK1 peptide or modified MEK2 peptide. In one embodiment, a method of growing crystals of a peptide: ligand: cofactor complex comprises providing an aqueous solution of a modified MEK1 or MEK2 peptide, a ligand and a cofactor in a solution of ammonium acetate and a N-2-hydroxyethyl-piperazine-N'-2-ethansulfonic acid (HEPES) buffer; providing a precipitant solution comprising (a) if the peptide is MEK1 peptide, polyethylene glycol (PEG), a source of ionic strength, a buffering agent, and a reducing agent; or (b) if the peptide is MEK2 peptide, a source of ionic strength, a buffering agent, and a reducing agent; mixing a droplet of said peptide solution with a droplet of said precipitant solution; suspending the resulting mixed droplet over a well of said precipitant solution at a vapor pressure of the solution in said well being lower than in the resulting solution in the mixed droplet; and allowing the suspended mixed droplet to stand for a prolonged period until a peptide: ligand: cofactor ternary complex crystal grows to a size suitable for X-ray diffraction. The MEK1 peptide may have a concentration from about 10 to about 20 mg/mL and the HEPES further may have a pH from about pH 7 to about pH 8. The MEK2 peptide may have a concentration from about 10 to about 20 mg/mL and the HEPES further may have a pH from about pH 6.8 to about pH 8.8.

[0024] The invention also provides the crystal structure of the modified MEK1 peptide in a ternary complex with ligands and cofactors, from which MEK1 structural information may be obtained. Preferably, the ligand is 5-bromo-N-(2,3-dihydroxy-propxy)-3,4-difluoro-2-(2-fluoro-4-iodo-phenylamino)-benzamide and the cofactor is ATP. The crystals preferably diffract to a resolution better than 5.0 Å, preferably 3.0 Å. The crystal structure of the modified MEK1 peptide: 5-bromo-N-(2,3-dihydroxy-propxy)-3,4-difluoro-2-(2-fluoro-4-iodo-phenylamino)-benzamide: ATP complex is the first reported of the MEK1 peptide or any of the related MAPKK family.

[0025] Additionally, the invention provides the crystal structure of the modified MEK2 peptide in a ternary complex with ligands and cofactors, from which the MEK2 structural information may be obtained. Preferably, the ligand is {5-[3,4-Difluoro-2-(2-fluoro-4-iodo-phenylamino)-phenyl]-1,3,4-oxadiazol-2-yl}-(2-morpholin-4-yl-ethyl)-amine and the cofactor is ATP. The crystals preferably diffract to a resolution better than 5.0 Å, preferably 3.5 Å. The crystal structure of the modified MEK2: {5-[3,4-Difluoro-2-(2-fluoro-4-iodo-phenylamino)-phenyl]-1,3,4-oxadiazol-2-yl}-(2-morpholin-4-yl-ethyl)-amine: ATP complex is the first reported of the MEK2 peptide family.

[0026] The invention further includes the three-dimensional structural coordinates of the MEK1 peptide and MEK2 peptide: ligand: cofactor complexes, as set forth in Tables 1 and 2, or of a related set of structural coordinates having a root mean square deviation of preferably not more than about 1.25 Å away from the core C alpha atoms of the MEK1 or MEK2 the three-dimensional structural coordinates as set forth in Table 1 or Table 2. The structural coordinates reflect the three-dimensional structure of the MEK1 complexes and MEK2 complexes and illustrates to atomic resolution the chemical environment around the MEK1 and MEK2 ligand- and cofactor-binding sites.

[0027] Particularly, it has been discovered that MEK1 comprises a peptide ligand-binding pocket that is defined by the structural coordinates of the following amino acid residues within about 4 Å of a MEK1 inhibitor located in the ligand-binding site: G77, N78, G79, G80, K97, I99, L115, L118, V127, F129, I141, M143, C207, D208, F209, G210, V211, S212, L215, I216 and M219 of SEQ ID NO: 2 or a conservatively substituted variant thereof; and is defined by the structural coordinates of the following amino acid residues within about 5 Å of a MEK1 inhibitor located in the ligand-

binding site: G77, N78, G79, G80, K97, I99, L115, L118, I126, V127, G128, F129, I141, M143, D190, N195, L206, C207, D208, F209, G210, V211, S212, L215, I216, M219 and F223 of SEQ ID NO: 2, or a conservatively substituted variant thereof.

[0028] It has also been discovered that MEK1 peptide comprises a cofactor-binding pocket that is defined by the structural coordinates of the following residues within about 4 Å of a cofactor (e.g. an ATP molecule) located in the cofactor-binding site: L74, G75, A76, G77, N78, G80, V81, V82, A95, K97, V127, M143, E144, H145, M146, G149, S150, D152, Q153, K192, S194, N195, L197, D208 and V224 of SEQ ID NO: 2, or a conservatively substituted variant thereof; and is defined by the structural coordinates of the following residues within about 5 Å of a cofactor located in the cofactor-binding site: L74, G75, A76, G77, N78, G79, 80, V81, V82, A95, K97, V127, M143, E144, H145, M146, D147, G149, S150, D152, Q153, D190, K192, S194, N195, L197, C207, D208, V224 and G225 of SEQ ID NO:2, or a conservatively substituted variant thereof.

[0029] Likewise, it has been discovered that MEK2 peptide comprises a ligand-binding pocket that is defined by the structural coordinates of the following amino acid residues within about 4 Å of a MEK2 inhibitor located in the ligand-binding site: G81, N82, G83, G84, K101, I103, L119, L122, V131, F133, I145, M147, C211, D212, F213, G214, V215, S216, L219, I220, M223 of SEQ ID NO: 4, or a conservatively substituted variant thereof; and is defined by structural coordinates of the following amino acid residues within about 5 Å of a MEK2 inhibitor located in the ligand-binding site: G81, N82, G83, G84, K101, I103, L119, L122, I130, V131, G132, F133, I145, M147, D194, N199, L210, C211, D212, F213, G214, V215, S216, L219, I220, M223, F227 of SEQ ID NO: 4, or a conservatively substituted variant thereof.

[0030] Additionally, it has been discovered that a MEK2 cofactor-binding pocket is defined by the structural coordinates of the following residues within about 4 Å of a cofactor located in the cofactor-binding site: L78, G79, A80, G81, N82, G84, V85, V86, A99, K101, V131, M147, E148, H149, M150, G153, S154, D156, Q157, K196, S198, N199, L201, D212, V228 of SEQ ID NO: 4, or a conservatively substituted variant thereof; and is defined by the structural coordinates of the following residues within about 5 Å of a cofactor located in the cofactor-binding site: L78, G79, A80, G81, N82, G83, G84, V85, V86, A99, K101, V131, M147, E148, H149, M150, D151, G153, S154, D156, Q157, D194, K196, S198, N199, L201, C211, D212, V228, G229 of SEQ ID NO: 4, or a conservatively substituted variant thereof.

[0031] A ligand- or cofactor-binding pocket of a MEK peptide or peptide that is structurally related to MEK1 or MEK2 peptide is also provided, wherein the ligandor cofactor-binding pocket is defined by the atoms found in the structural coordinates of the MEK1 or MEK2 peptide as set forth in Table 1 or Table 2, or in a related set of structural coordinates having a root mean square deviation of not more than preferably about 1.25 Å away from the binding pocket C alpha atoms of a MEK1 or MEK2 binding pockets.

[0032] The invention also provides a machine-readable medium having stored thereon data comprising the atomic coordinates as set forth in Table 1 or Table 2, or a related set of structural coordinates having a root mean square deviation of not more than preferably about 1.25 Å away from the core C alpha atoms of the MEK1 or MEK2 structural coordinates as set forth in Table 1 or Table 2

[0033] The invention also provides for applying the the atomic coordinates set forth in Table 1 or Table 2, or of a related set of atomic coordinates having a root mean square deviation of not more than preferably about 1.25 Å away from the core C alpha atoms of the MEK1 or MEK2 structural coordinates as set forth in Table 1 or Table 2, to a computer algorithm to generate a three-dimensional representation (also referred to as an "image") of a peptide or peptide binding pocket of the invention. This three-dimensional represenation can be used, for example, in methods for modifying, designing, screening and identifying, and evaluating chemical entities that have the potential to associate with MEK1, MEK2, or a structurally related peptide, and thus have the potential to be an inhibitor or enhancer of MEK1, MEK2, or a structurally related peptide.

[0034] Additionally, the invention provides methods for modifying or designing a chemical entity having the potential to associate with a peptide of the invention. The methods include generating a three-dimensional computer representation of the peptide or a binding pocket of the peptide and generating a chemical entity that spatially conforms to the three-dimensional representation of the peptide or the peptide binding pocket. The chemical entity may be generated by a method comprising (i) assembling molecular fragments into the chemical entity; (ii) de novo design of the chemical entity or a fragment thereof; (iii) selecting the chemical entity from a small molecule database; or (iv) modifying a known inhibitor, or portion thereof, which possess the ability to associate with either MEK1, MEK2 or the structurally related peptide.

[0035] The invention also provides methods for screening and identifying a potential inhibitor or enhancer of the activity of a peptide of the invention. The methods include generating a three-dimensional computer representation of the peptide or a binding pocket of the peptide; applying an iterative process whereby a chemical entity is applied to the three-dimensional representation to determine whether the chemical entity associates with the peptide or peptide binding pocket; and evaluating the effect(s) of the chemical entity on peptide activity to determine whether the chemical entity functions as an activity inhibitor or enhancer.

[0036] Methods for evaluating the potential of a chemical entity to associate with a peptide according to the invention are also provided. The methods include generating a three-dimensional representation of the peptide or a binding

pocket of the peptide; applying a three-dimensional representation of chemical entity to the three-dimensional representation; and quantifying the association between the chemical entity and the binding pocket.

[0037] Additionally, the invention provides methods of utilizing molecular replacement to obtain structural information about a molecule or a molecular complex of unknown structure comprising crystallizing said molecule or molecular complex; generating an X-ray diffraction pattern from said crystallized molecule or molecular complex; and applying at least a portion of the structural coordinates set forth in Table 1 or Table 2 or having a set of structural coordinates with a root mean square deviation of preferably not more than about 1.25 Å from the core C alpha atoms of the MEK1 or MEK2 structural coordinates as set forth in Table 1 or Table 2, to the X-ray diffraction pattern to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown.

BRIEF DESCRIPTION OF THE DRAWINGS

[0038] The application file contains at least one drawing executed in color. Copies of the patent application publication with color drawings will be provided by the Office upon request and payment of the necessary fee.

[0039] **Figure 1.** Figure 1 is a ribbon representation of the three-dimensional structure of the NH_2-terminally truncated MEK1 peptide structure, in a ternary complex with 5-bromo-N-(2,3-dihydroxy-propxy)-3,4-difluoro-2-(2-fluoro-4-iodo-phenylamino)-benzamide and MgATP. The alpha helical regions of the peptide are colored blue, the beta sheet regions are colored green, the ATP co-factor is purple, the magnesium atom is colored cyan and the inhibitor is colored red. The Mg-ATP molecule is bound at the active site cleft between the NH_2- and COOH-terminal lobes as found in other kinase structures, while the inhibitor binds in a pocket at the back of the cleft formed in part by the activation loop.

[0040] **Figure 2.** Figure 2 is a ribbon representation of the three-dimensional structure of the NH_2-terminally truncated MEK2 peptide structure, in a ternary complex with {5-[3,4-Difluoro-2-(2-fluoro-4-iodo-phenylamino)-phenyl]-1,3,4-oxadiazol-2-yl}-(2-morpholin-4-yl-ethyl)-amine and MgATP. The alpha helical regions of the peptide are colored blue, the beta sheet regions are colored green, the ATP co-factor is purple, the magnesium atom is colored cyan and the inhibitor is colored red. The MgATP molecule is bound at the active site cleft between the NH_2-and COOH-terminal lobes as found in other kinase structures, while the inhibitor binds in a pocket at the back of the cleft formed in part by the activation loop.

[0041] **Figure 3.** Figure 3 is superposition of the three-dimensional structures of MEK1 (blue) and MEK2 (red) peptides using the C alpha atoms of commonly observed residues.

[0042] **Figure 4.** Figure 4 illustrates the interactions involved in the orientation of the ligand (referred to as "pd0318088" in the figure) within the MEK1 active site. The back right side of the figure shows the H-donor and acceptor bond formed between the backbone nitrogen of Ser212 and the 4-fluoro group of the inhibitor. Also shown at the top of the figure is the iodine of the inhibitor forming an electrostatic interaction with the backbone carbonyl of Val127. Finally, Leu115, Leu118 and Phe209 participate in forming the prime hydrophobic pocket.

[0043] **Figure 5.** Figure 5 illustrates the interactions involved in the orientation of the ligand (referred to as "PD0334581" in the figure) within the MEK2 active site. The back right side of the figure shows the H-donor and acceptor bond formed between the backbone nitrogen of Ser216 and the 4-fluoro group of the inhibitor. Also shown at the top of the figure is the iodine of the inhibitor forming an electrostatic interaction with the backbone carbonyl of Val131. Finally, Leu119, Leu122 and Phe213 participate in forming the prime hydrophobic pocket.

SEQUENCE LISTING

SEQ ID NO: 1 Full-length of MEK1 nucleotide

SEQ ID NO: 2 Full-length of MEK1 peptide

SEQ ID NO: 3 Full-length of MEK2 nucleotide

SEQ ID NO: 4 Full-length of MEK2 peptide

SEQ ID NO: 5 Probe for MEK1

SEQ ID NO: 6 Probe for MEK1

SEQ ID NO: 7 PCR primer for MEK1-C1/MEK1-C1(d280-323)

SEQ ID NO: 8 PCR primer for MEK1-C1/MEK1-C1(d280-323); MEK1-C2/MEK1-C2(d280-323); and PCR primer for MEK1-C3/MEK1-C3(d280-323)

SEQ ID NO: 9 PCR primer for MEK1-C2/MEK1-C2(d280-323)

SEQ ID NO: 10 PCR primer for MEK1-C3/MEK1-C3(d280-323)

SEQ ID NO: 11 PCR probe for MEK2

SEQ ID NO: 12 PCR probe for MEK2

SEQ ID NO: 13 PCR primer for MEK2-C1

SEQ ID NO: 14 PCR primer for MEK2-C2

SEQ ID NO: 15 PCR primer for MEK2-C3

SEQ ID NO: 16 PCR primer for MEK2-C4

SEQ ID NO: 17 PCR primer for MEK2-C5

SEQ ID NO: 18 PCR primer for MEK2-C6

SEQ ID NO: 19 PCR reverse primer for MEK2-C1-C6

DETAILED DESCRIPTION OF PREFERRED EMBODIMENTS

[0044] The present invention provides modified MEK1 and modified MEK2 peptides, and crystals of a peptide: ligand: cofactor complex that preferably comprise a ternary (i.e. tertiary) complex of a modified MEK1 peptide or modified MEK2 peptide, or a peptide that is structurally related to MEK1 or MEK2 peptide, a ligand and a cofactor.

[0045] According to one embodiment of the invention, the crystals are formed from recombinant human MEK1 peptide or recombinant human MEK2 peptide derived from a circular nucleic acid sequence that preferably has been expressed in a prokaryotic host and purified. The crystals diffract X-rays to a resolution better than 5Å. The information derived from the crystals provides three-dimensional crystallographic structural information for the MEK1 complex and the MEK2 complex, including ligand-binding and cofactor-binding sites of the MEK1 peptide, MEK2 peptide or a peptide that is structurally related to MEK1 or MEK2 peptide. The present invention includes the use of this structural information in, for example, the modification, design, screening and identification, and evaluation of chemical entities that have the potential to associate with MEK1 or MEK2 peptide, or a peptide that is structurally related thereto, and thus may inhibit or enhance MEK1 or MEK2 activity.

Defintions

[0046] As used herein, the terms "comprising" and "including" are used in the conventional, non-limiting sense.

[0047] As used herein, "ligand" means a small molecule that binds to or associates specifically with an enzyme and can be used to mean an inhibitor or an activator.

[0048] As used herein, "cofactor" means an inorganic molecule, an organic molecule or a coenzyme that is required for enzymatic activity. For example, ATP (adenosine triphosphate) is a cofactor used by a kinase enzyme to transfer a phosphate group, i.e. phosphorylate its substrate.

[0049] As used herein, the phrase "root mean square (RMS) deviation" denotes the structural relationship between two or more species of proteins or peptides. It means that the difference in the root mean square of the distance of the three-dimensional structure of one peptide from C-alpha (C_α) atoms or backbone trace of the MEK1 peptide or MEK2 peptide in units of Angstroms (Å) unless indicated otherwise. It may be determined by superimposing one of the three-dimensional structures of the species on another, which may be solved by, for example, X-ray crystallography or by NMR and measuring the difference in the root mean square of the distance from C_α atoms or backbone trace of the MEK1 or MEK2 peptide to the other peptide in units of Angstroms (Å). The superimposing of three-dimensional structures on one another may be performed using a molecular modeling program, for example CNX™ (Accelrys), XtalView™ (Duncan McRee, Scripps Research Institute) or O™ (Morten Kjeldgaard, Aarhus Univ., Denmark). The closer the relationship between the three-dimensional structures, the smaller will be the value of the RMS deviation. For example, the three-dimensional relationship between the structural coordinates of the C-alpha atoms of two ligand protein co-complex structures is typically between 0.0 - 0.5 Å RMS deviation. An example of the caulation of a RMS deviation, specifically between the MEK1 and MEK2 crystalline structures of the invention, is provided herein in Example 16.

[0050] Therefore, one embodiment of this invention is the three-dimensional structures of the modified MEK1 and MEK2 peptides in ternary complexes with a ligand and a cofactor as found in Table 1 and Table 2. An additional embodiment is a "structurally related" peptide, crystals of the structurally related peptide and the three-dimensional structures thereof.

[0051] As used herein, a "structurally related" protein or peptide refers to a protein or peptide that is defined by the structural coordinates of the MEK1 or MEK2 peptide as set forth in Table 1 or Table 2 or a related set of structural coordinates having a root mean square deviation of from not more than about 1.5 Å to not more than about 0.50 Å from the core C alpha atoms of the MEK1 or MEK2 peptide structural coordinates as set forth in Table 1 or Table 2. Preferably the root mean square deviation is not more than about 0.50Å, more preferably not more than about 0.75 Å, even more preferably not more than about 1.00 Å, and most preferably not more than about 1.25 Å. An example of such a "structurally related peptide" may be, but is not limited to, MEK5.

[0052] Similarly, as used herein, "related set of structural coordinates" refers to a set of structural coordinates having a root mean square deviation in the range of from not more than about 1.5 Å to not more than about 0.50 Å away from the core C alpha atoms of the MEK1 or MEK2 structural coordinates a set forth in Table 1 or Table 2. Preferably the root mean square deviation is not more than about 0.50Å, more preferably not more than about 0.75 Å, even more preferably not more than about 1.00 Å, and most preferably not more than about 1.25 Å.

[0053] As used herein, "chemical entity" refers to a chemical compound, a complex of at least two chemical compounds, or a fragment of such a compound or complex. Such entities can be, for example, potential drug candidates and can be evaluated for their ability to inhibit or enhance the activity of MEK1, MEK2, or a structurally related peptide.

[0054] As used herein, the term "inhibitor" or "inhibit" (or variations thereof) refers to a ligand such as a compound or substance that lowers, reduces, decreases, prevents, diminishes, stops or negatively interferes with MEK1's or MEK2's activity, or such actions. Often the terms "inhibitor" and "antagonists" can be used interchangeably. Inhibition is typically expressed as a percentage of the enzymes activity in the presence of the inhibitor over the enzymes activity without the inhibitor. Or it may be expressed in terms of IC50, the inhibitor concentration at which 50% of the original enzyme activity is observed.

[0055] As used herein, the term "enhancer" or "enhance" (or variations thereof) refers to a ligand such as a compound or substance that improves, increases, stimulates, raises or positively interferes with MEK1 or MEK2 activity, or such actions. Often the terms "enhancer" or "agonists" can be used interchangeably. An enhancer would increase the enzyme's activity.

[0056] As used herein, the terms "model" and "modeling" mean the procedure of evaluating (also referred to as "assessing") the affinity of the interaction between a MEK1, MEK2, MEK-like binding pocket and a chemical entity (also referred to as a "candidate compound") based on steric constraints and surface/solvent electrostatic effects.

MEK1 and MEK2

[0057] As used herein, the abbreviation "MEK1" or "Mek1" refers to the polynucleotide encoding the MAP kinase

/ERK1 kinase, or the peptide *per se*. The MEK1 peptide is sometimes referred to as MAPKK, MPK1, MEK1, MAP kinase kinase 1 or MAP kinase /ERK1 kinase in the literature and throughout this application. The nucleic acid sequence of the polynucleotide encoding the full-length protein of MEK1 was published by Zheng and Guan (*J. Biol. Chem.* 268, 11435-11439 (1993)) and submitted to GenBank under the accession number L11284. The nucleic acid sequence described therein is provided herein, shown in SEQ ID NO: 1. The corresponding peptide sequence of the full-length protein is provided herein, shown in SEQ ID NO: 2. This peptide sequence was submitted to GenBank by Zheng *et al.* and Seger *et al.* and assigned Accession number NP_002746. It is noted that the numbering of SEQ ID NO:2 provided herein begins at the starting codon ATG (Met).

[0058] As used herein, the abbreviation "MEK2" or Mek2" refers to the polynucleotide encoding the MAP kinase kinase 2 or MAP Kinase/ ERK2 kinase, or the peptide *per se.* The MEK2 peptide is sometimes also referred to as MAPKK2 or MPK2. MEK2 is a paralog of MEK1 in the literature and throughout this application. MEK2 peptide, and the polynucleotide encoding the full-length MEK2 peptide were reported by Zheng *et al.* (*J. Biol. Chem.* 268, 11435-11439 (1993)) and their sequences are available under GenBank Accession numbers P36507 and NM_030662, respectively. The nucleic acid sequence encoding MEK2 and amino acid sequence of MEK2 peptide are provided herein as SEQ ID NO: 3 and SEQ ID NO: 4, respectively.

MEK1 and MEK2 Peptide Binding Pockets

[0059] As used herein, "binding pocket," also referred to as, for example, "binding site," "binding domain," "substrate-binding site," "catalytic domain," or "ligand-binding domain," "ligand-binding site," "co-factor-binding site," or "co-factor-binding domain," refers to a region or regions of a molecule or molecular complex, that, as a result of its surface features, including, but not limited to, volume (both internally in cavities or in total), solvent accessibility, and surface charge and hydrophobicity, can associate with another chemical entity or compound. Such regions are of utility in fields such as drug discovery.

[0060] As used herein, a "MEK-like" peptide binding pocket refers to a peptide binding pocket defined by the atoms found in the structural coordinates of the MEK1 or MEK2 peptide as set forth in Table 1 or Table 2, or defined by structural coordinates having a root mean square deviation ranging from not more than about 1.5 Å to not more than about about 0.50 Å, preferably of not more than about 1.25 Å, away from the binding pocket C alpha atoms of any one of the MEK1 or MEK2 binding pockets (e.g. the MEK1 or MEK2 cofactor or ligand binding pockets defined above in the Summary of the Invetion section), or a conservatively substituted variant thereof.

[0061] As used herein, the term "activity" refers to all activities, i.e., the function of MEK1 or MEK2 in the phosphorylation of its substrate ERK1, as well as to the enzymes' potency. Often the terms "activity" and "'function" can be used interchangeably.

[0062] As used herein, the term "associate" refers to the process in which at least two molecules reversibly interact with each other, for example, by binding with each other. This may also refer to the process in which the conformation of the protein changes in response to the presence of a ligand to better accommodate the steric and electrostatic effects of the ligand. Associations between MEK1, MEK2, or a structurally related peptide and a ligand may occur with all or a part of a MEK1, MEK2, or MEK-like binding pocket. The association(s) may be non-covalent, e.g., wherein the juxtaposition is energetically favored by hydrogen bonding, van der Waals interactions or electrostatic interactions, or the association(s) may be covalent.

MEK1 and MEK2 Peptides

[0063] The present invention provides isolated peptides and protein molecules that consist of, consist essentially of or are comprised of the amino acid sequences of the peptides encoded by the nucleic acid sequences disclosed in the SEQ ID NO: 1 and SEQ ID NO: 3, as well as obvious variants of these peptides that the within the art to make and use. Some of these variants are described in detail below.

Modified MEK1 Peptide

[0064] In one embodiment, the invention provides an isolated, substantially pure polypeptide comprising novel modified MEK1 peptides, constructed, for example, so as to omit a significant portion of the flexible NH_2-terminal tail, or a conservatively substituted variant thereof ("NH_2-terminally truncated MEK1 peptides"). The NH_2-terminally truncated MEK1 peptide of the present invention preferably retains the globular core of the corresponding full-length of MEK1 peptide, such that MEK1 peptide can bind to ATP, its natural cofactor. Preferably, the NH_2-terminally truncated MEK1 peptides lack all or a significant portion (minimally 30 amino acids, preferably 41 amino acids, more preferably up to 50 amino acids, and even more preferably up to 61 amino acids) of the flexible, partially disordered NH_2-terminus which includes a portion of the ERK1 binding domain. In addition, the NH_2-terminally truncated MEK1 peptides may

have a methionine as the initial amino acid prior to the indicated sequence.

[0065] These NH_2-terminally truncated MEK1 peptide may further have a deletion of the MEK1 insertion loop-forming domain, particularly from amino acid 280 to 323 of SEQ ID NO: 2 or at least 40 amino acids from between 264 and 310 of SEQ ID NO: 2. This may include a deletion of amino acids (1) from amino acid 264 to amino acid 310 of SEQ ID NO: 2; (2) from amino acid 270 to amino acid 310 of SEQ ID NO: 2; (3) from amino acid 264 to amino acid 305 of SEQ ID NO: 2; (4) amino acid 267 to amino acid 307 of SEQ ID NO: 2; or (5) from amino acid 265 to amino acid 304 of SEQ ID NO: 2.

[0066] The MEK1 insertion loop domain may also be replaced with a linker peptide. Preferably, the linker peptide has at most 10 amino acid residues. More preferably, the linker peptide has the amino acid sequence Lys-Asn-Cys-Lys-Thr-Asp.

[0067] Alternatively, the MEK1 peptide may be modified by a deletion of the MEK1 insertion loop-forming domain and/or by replacement of the MEK1 insertion loop domain as described above, without NH_2-terminal truncation.

[0068] These modified MEK1 peptides may also have a histidine oligomer tag, for example a histidine hexamer tag (His-Tag) at its COOH-terminus.

[0069] For example, the modified MEK1 peptide can be chosen from any of the following: (1) a NH_2-terminally truncated MEK1 peptide comprising amino acids 62-393 of the sequence shown in SEQ ID NO: 2, optionally containing a COOH-terminal His-Tag; (2) a NH_2-terminally truncated MEK1 peptide comprising amino acids 62-393 of SEQ ID NO: 2 with an additional deletion of insertion loop-forming amino acid residues as described above, and optionally containing a COOH-terminal His-Tag; (3) a NH_2-terminally truncated MEK1 peptide comprising amino acids 51-393 of the sequence shown in SEQ ID NO: 2, optionally containing a COOH-terminal His-Tag; (4) a NH_2-terminally truncated MEK1 peptide comprising amino acids 51-393 of SEQ ID NO: 2 with an additional deletion of insertion loop-forming amino acid residues as described above, and optionally containing a COOH-terminal His-Tag; (5) a NH_2-terminally truncated MEK1 peptide comprising amino acids 42-393 of the sequence shown in SEQ ID NO: 2, and which may optionally contain a COOH-terminal His-Tag; (6) a NH_2-terminally truncated MEK1 peptide comprising amino acids 42-393 of SEQ ID NO: 2 with an additional deletion of insertion loop-forming amino acid residues as described above, and optionally containing a COOH-terminal His-Tag; (7) a MEK1 peptide modified to have a deletion of insertion loop-forming amino acid residues as described above; and (8) a MEK peptide modified to replace the insertion loop-forming amino acid residues with a linker peptide, preferably Lys-Asn-Cys-Lys-Thr-Asp, with or without NH_2-terminal truncation described above.

[0070] Preferably, the modified MEK1 peptides retain the conserved amino acids described below and comprises approximately 331 to 351 amino acids residues, or approximately 284 to 311 amino acid residues if the NH_2-terminally truncated MEK1 peptides have a deletion within the peptide. The modified MEK1 peptide can be either phosphorylated or unphosphorylated. Similarly the modified MEK1 peptide can comprise one or more selenomethionines substituted for a naturally occurring methionine of the corresponding full-length MEK1 peptide. Of course, general modifications such as additional heavy atom derivatives common in X-ray crystallographic studies may also be performed on the modified MEK1 peptide of the present invention and such modifications are also included as part of the present inventions.

[0071] In a preferred embodiment, the modified MEK1 peptide is derived from human MEK1 and lacks the residues from amino acid 1 to amino acid 41 of the N-terminal amino acids of the corresponding full-length MEK1. In a more preferred embodiment, the modified MEK1 peptide lacks the residues from amino acid 1 to amino acid 50 of the N-terminal amino acids of the corresponding full-length MEK1. In the most preferred embodiment, the modified MEK1 peptide lacks the residues from amino acid 1 to amino acid 61 of the N-terminal amino acids of the corresponding full-length MEK1 shown in SEQ ID NO: 2.

[0072] The modified MEK1 peptides of the present invention can be derived from any eukaryotic source, but is preferably a vertebrate MEK1, more preferably from a mammalian MEK1, and most preferably human MEK1.

Modified MEK2 Peptide

[0073] In another embodiment, the invention provides an isolated, substantially pure polypeptide comprising novel modified MEK2 peptides, constructed, for example, so as to omit a significant portion of the flexible NH_2-terminal tail, or a conservatively substituted variant thereof ("NH_2-terminally truncated MEK2 peptides"). The NH_2-terminally truncated MEK2 peptide of the present invention preferably retains the globular core of the corresponding full-length of MEK2 peptide, such that MEK2 peptide can bind to ATP, its natural cofactor. Preferably, the NH_2-terminally truncated MEK2 peptides lack all or a significant portion (minimally 34 amino acids to at most 74 amino acids, preferably minimally 45 to at most 65 amino acids) of the flexible, partially disordered NH_2-terminus which includes a portion of the ERK2 binding domain. In addition, the NH_2-terminally truncated MEK2 peptides may have a methionine as the initial amino acid prior to the indicated sequence. These modified MEK2 peptides may also have a histidine oligomer tag, for example a histidine hexamer tag (His-Tag) at its COOH-terminus.

[0074] For example, the modified MEK2 peptide can be chosen from any of the following: (1) a NH_2-terminally truncated MEK2 peptide comprising amino acids 46-400 of the sequence shown in SEQ ID NO: 4, optionally containing a COOH-terminal His-Tag; (2) a NH_2-terminally truncated MEK2 peptide comprising amino acids 55-400 of the sequence shown in SEQ ID NO: 4, optionally containing a COON-terminal His-Tag; (3) a NH_2-terminally truncated MEK2 peptide comprising amino acids 66-400 of the sequence shown in SEQ ID NO: 4, and which may optionally contain a COOH-terminal His-Tag; (4) a NH_2-terminally truncated MEK2 peptide comprising amino acids 59-400 of the sequence shown in SEQ ID NO: 4, and which may optionally contain a COOH-terminal His-Tag; (5) a NH_2-terminally truncated MEK2 peptide comprising amino acids 62-400 of the sequence shown in SEQ ID NO: 4, and which may optionally contain a COOH-terminal His-Tag; (6) a NH_2-terminally truncated MEK2 peptide comprising amino acids 64-400 of the sequence shown in SEQ ID NO: 4, and which may optionally contain a COOH-terminal His-Tag.

[0075] Preferably, the modified MEK2 peptides retain the conserved amino acids described below and comprises approximately 326 to 366 amino acids residues. The modified MEK2 peptide can be either phosphorylated or unphosphorylated. Similarly the modified MEK2 peptide can comprise one or more selenomethionines substituted for a naturally occurring methionine of the corresponding full-length MEK2 peptide. Of course, general modifications such as additional heavy atom derivatives common in X-ray crystallographic studies may also be performed on the modified MEK2 peptide of the present invention and such modifications are also included as part of the present inventions.

[0076] In a preferred embodiment, the modified MEK2 peptide is derived from human MEK2 and lacks the residues from amino acid 1 to amino acid 45 of the N-terminal amino acids of the corresponding full-length MEK2 shown in SEQ ID NO: 4. In a more preferred embodiment, the modified MEK2 peptide lacks the residues from amino acid 1 to amino acid 54 of the N-terminal amino acids of the corresponding full-length MEK2 shown in SEQ ID NO: 4. In the most preferred embodiment, the modified MEK2 peptide lacks the residues from amino acid 1 to amino acid 65 of the N-terminal amino acids of the corresponding full-length MEK2 shown in SEQ ID NO: 4.

[0077] The modified MEK2 peptides of the present invention can be derived from any eukaryotic source, but is preferably a vertebrate MEK2, more preferably from a mammalian MEK2, and most preferably human MEK2.

[0078] As used herein, a protein or peptide is said to be "isolated" or "purified" when it is substantially free of cellular material or free of chemical precursors or other chemicals. The proteins or peptides of the present invention can be purified to homogeneity or other degrees of purity. The level of purification will be based on the intended use. The critical feature is that the preparation allows for the desired function of the protein or peptide, even if in the presence of considerable amounts of other components.

[0079] In some uses, "substantially free of cellular material" includes preparations of the protein or peptide having less than about 30% (by dry weight) other proteins (i.e., contaminating protein), preferably less than about 20% other proteins, more preferably less than about 10% other proteins, or even more preferably less than about 5% other proteins. When the protein or peptide is recombinantly produced, it can also be substantially free of culture medium, i.e., culture medium represents less than about 20% of the volume of the protein preparation.

[0080] The language "substantially free of chemical precursors or other chemicals" includes preparations of the protein in which it is separated from chemical precursors or other chemicals that are involved in its synthesis. In one embodiment, the language "substantially free of chemical precursors or other chemicals" includes preparations of the protein having less than about 30% (by dry weight) chemical precursors or other chemicals, preferably less than about 20% chemical precursors or other chemicals, more preferably less than about 10% chemical precursors or other chemicals, or most preferably less than about 5% chemical precursors or other chemicals.

[0081] The isolated protein described herein can be purified from cells that naturally express MEK1 or MEK2 peptide or purified from cells that have been altered to express MEK1 or MEK2 (recombinant expression). For example, a nucleic acid molecule encoding the protein is cloned into an expression vector, the expression vector is introduced into a host cell and the protein is then expressed in the host cell. The protein can then be isolated from the cells by an appropriate purification scheme using standard protein purification techniques. Many of these techniques are described in detail below.

[0082] "Polypeptide" refers to any peptide or protein comprising two or more amino acids joined to each other by peptide bonds or modified peptide bonds, i.e., peptide isosteres. "Polypeptide" refers to both short chains, commonly referred to as peptides, oligopeptides or oligomers, and to longer chains, generally referred to as proteins. The terms "peptide", "polypeptide" and "protein" are used interchangeably herein. Polypeptides may contain amino acids other than the 20 naturally occurring amino acids. Further, many amino acids, including the terminal amino acids, may be modified by natural processes, such as processing and other post-translational modifications, or by chemical modification techniques well known in the art. Common modifications that occur naturally in polypeptides are described in basic texts, detailed monographs, and the research literature, and they are well known to those of skill in the art.

[0083] Accordingly, the polypeptides also encompass derivatives or analogs in which a substituted amino acid residue is not one encoded by the genetic code; in which a substituent group is included, in which the mature polypeptide is fused with another compound, such as a compound to increase the half-life of the polypeptide (for example, polyethylene glycol), or in which the additional amino acids are fused to the mature polypeptide, such as a leader or secretary

sequence or a sequence for purification of the mature polypeptide or a pro-protein sequence.

[0084] The present invention further provides for fragments of the MEK1 and MEK2 peptides, in addition to proteins and peptides that comprises and consist of such fragments. As used herein, a fragment comprises at least 8 or more contiguous amino acid residues from the protein kinase. Such fragments can be chosen based on the ability to retain one or more of the biological activities of the kinase or could be chosen for the ability to perform a function, e.g. act as an immunogen. Particularly important fragments are biologically active fragments, peptides which are, for example about 8 or more amino acids in length. Such fragments will typically comprise a domain or motif of the kinase, e.g., active site. Further, possible fragments include, but are not limited to, domain or motif containing fragments, soluble peptide fragments, and fragments containing immunogenic structures. Predicted domains and functional sites are readily identifiable by computer programs well known and readily available to those of skill in the art (e.g., by PROSITE analysis).

[0085] Known modifications include, but are not limited to, acetylation, acylation, ADP-ribosylation, amidation, covalent attachment of flavin, covalent attachment of a heme moiety, covalent attachment of a nucleotide or nucleotide derivative, covalent attachment of a lipid or lipid derivative, covalent attachment of phosphotidylinositol, cross-linking, cyclization, disulfide bond formation, demethylation, formation of covalent crosslinks, formation of cystine, formation of pyroglutamate, formylation, gamma carboxylation, glycosylation, GPI anchor formation, hydroxylation, iodination, methylation, myristoylation, oxidation, proteolytic processing, phosphorylation, phenylation, racemization, selenoylation, sulfation, transfer-RNA mediated addition of amino acids to proteins such as arginylation, and ubiquitination.

[0086] Such modifications are well known to those of skill in the art and have been described in great detail in the scientific literature. Several particularly common modifications, glycosylation, lipid attachment, sulfation, gamma-carboxylation of glutamic acid residues, hydroxylation and ADP-ribosylation, for instance, are described in most basic texts. For example, see *Proteins - Structure and Molecular Properties,* 2nd Ed., T.E. Creighton, W. H. Freeman and Company, New York (1993). Many detailed reviews are available on this subject, such as by Wold, F., *Posttranslational Covalent Modification of Proteins,* B.C. Johnson, Ed., Academic Press, New York 1-12 (1983); Seifter *et al.* (*Meth. Enzymol. 182*: 626-646 (1990)) and Rattan *et al.* (*Ann. N.Y. Acad. Sci. 663: 48-62* (1992)).

[0087] The peptides of the present invention can be attached to heterologous sequences to form chimeric or fusion proteins. Such chimeric and fusion proteins comprise a peptide operatively linked to a heterologous protein having an amino acid sequence not substantially homologous to the kinase peptide. "Operatively linked" indicates that the peptide and the heterologous protein are fused in-frame. The heterologous protein can be fused to the NH_2-terminus or COOH-terminus of the kinase peptide. The two peptides linked in a fusion peptide are typically derived from two independent sources, and therefore a fusion peptide comprises two linked peptides not normally found linked in nature. The two peptides may be from the same or different genome.

[0088] In some uses, the fusion protein does not affect the activity of the peptide *per se.* For example, the fusion protein can include, but is not limited to, enzymatic fusion proteins, for example beta-galactosidase fusions, yeast two-hybrid GAL fusions, poly-His fusions, MYC-tagged, HI-tagged and Ig fusions. Such fusion proteins, particularly poly-His fusions, can facilitate the purification of recombinant kinase peptide. In certain host cells (e.g., mammalian host cells), expression and/or secretion of a protein can be increased by using a heterologous signal sequence.

[0089] A chimeric or fusion protein can be produced by standard recombinant DNA techniques. For example, DNA fragments coding for the different protein sequences are ligated together in-frame in accordance with conventional techniques. In another embodiment, the fusion gene can be synthesized by conventional techniques including automated DNA synthesizers. Alternatively, PCR amplification of gene fragments can be carried out using anchor primers which give rise to complementary overhangs between two consecutive gene fragments which can subsequently be annealed and reamplified to generate a chimeric gene sequence (see Ausubel *et al., Current Protocols in Molecular Biology*, 1992). Moreover, many expression vectors are commercially available that already encode a fusion moiety (e.g., a GST protein). A modified MEK1 peptide-encoding nucleic acid can be cloned into such an expression vector such that the fusion moiety is linked in-frame to the peptide.

Nucleic Acids and Polynucleotides Encoding Modified MEK1 and MEK2 Peptides

[0090] The present invention also provides isolated nucleic acid molecules that encode the functional, active kinases of the present invention. Such nucleic acid molecules will consist of, consist essentially of, or comprise a nucleotide sequence that encodes one of the kinase peptides of the present invention, an allelic variant thereof, or an ortholog or paralog thereof.

Polynucleotides Encoding Modified MEK1 Peptides

[0091] In a particular embodiment, the invention also provides isolated, purified polynucleotides that encode novel modified MEK1 peptides, such as NH_2-terminally truncated MEK1 peptides, MEK1 peptides having a deletion of in-

sertion loop-forming domains, and/or MEK1 having the insertion loop domain replaced with a linker peptide.

[0092] The polynucleotide may be natural or recombinant. In one embodiment, the nucleic acid sequence encodes a modified MEK1 peptide having an amino acid sequence of amino acids from between amino acids 42 and 62 to amino acid 393 of SEQ ID NO: 2 or a conservatively substituted variant thereof. In particular, the nucleic acid sequence encodes a modified MEK1 peptide having an amino acid sequence of amino acids 42 to 393 of SEQ ID NO: 2 or an amino acid sequence that differs from amino acid 42 to 393 of SEQ ID NO: 2 by only having conservative substitutions. Alternatively, the nucleic acid sequence encodes a modified MEK1 peptide having an amino acid sequence of amino acids 51 to 393 of SEQ ID NO: 2 or an amino acid sequence that differs from amino acid 51 to 393 of SEQ ID NO: 2 by only having conservative substitutions. Or, the nucleic acid sequence encodes a modified MEK1 peptide having an amino acid sequence of amino acids 62 to 393 of SEQ ID NO: 2 or an amino acid sequence that differs from amino acid 62 to 393 of SEQ ID NO: 2 by only having conservative substitutions. Such polynucleotides may be, for example, one having the sequence set forth in SEQ ID NO: 1 with deletion of the portion encoding the first 41-61 amino residues of the sequence of SEQ ID NO: 2.

[0093] In addition, the polynucleotide may encode the modified MEK1 peptide to further have a deletion of insertion loop-forming domain, particularly from amino acid 280 to 323 of SEQ ID NO: 2; or at least 40 amino acids from between amino acid residue 264 and amino acid 310 of SEQ ID NO: 2. This may include a deletion of amino acids (1) from amino acid 264 to amino acid 310 of SEQ ID NO: 2; (2) from amino acid 270 to amino acid 310 of SEQ ID NO: 2; (3) from amino acid 264 to amino acid 305 of SEQ ID NO: 2; (4) amino acid 267 to amino acid 307 of SEQ ID NO: 2; or (5) from amino acid 265 to amino acid 304 of SEQ ID NO: 2.

[0094] Moreover, the polynucleotide may encode the MEK1 peptide modified to replace the MEK1 insertion loop-forming amino acid residues with a linker peptide, preferably Lys-Asn-Cys-Lys-Thr-Asp, either alone or in combination with the NH_2-terminal truncations described above.

[0095] The polynucleotide of the invention also may encode the MEK1 peptides modified to have a deletion of insertion loop-forming amino acid residues as described above, without NH_2-terminal truncation.

[0096] Also, any of these amino acid sequences may contain one or more selenomethionines in place of a methionine. Further, these modified MEK1 peptides and their various variants may have a histidine oligomer tag, for example a histidine hexamer tag (His-tag) at their COOH-terminus.

Polynucleotides Encoding Modified MEK2 Peptides

[0097] In another particular embodiment, the invention also provides isolated, purified polynucleotides that encode novel modified MEK2 peptides, such as NH_2-terminally truncated MEK2 peptides. The polynucleotide may be natural or recombinant. In one embodiment, the nucleic acid sequence encodes a modified MEK2 peptide having an amino acid sequence of amino acids from between amino acids 46 and 66 to amino acid 400 of SEQ ID NO: 4 or a conservatively substituted variant thereof. In particular, the nucleic acid sequence encodes a modified MEK2 peptide having an amino acid sequence of amino acids 46 to 400 of SEQ ID NO: 4 or an amino acid sequence that differs from amino acid 46 to 400 of SEQ ID NO: 4 by only having conservative substitutions. Alternatively, the nucleic acid sequence encodes a modified MEK2 peptide having an amino acid sequence of amino acids 55 to 400 of SEQ ID NO: 4 or an amino acid sequence that differs from amino acid 55 to 400 of SEQ ID NO: 4 by only having conservative substitutions. Or, the nucleic acid sequence encodes a modified MEK2 peptide having an amino acid sequence of amino acids 66 to 400 of SEQ ID NO: 4 or an amino acid sequence that differs from amino acid 66 to 400 of SEQ ID NO: 4 by only having conservative substitutions. Alternatively, the nucleic acid sequence encodes a modified MEK2 peptide having an amino acid sequence of amino acids 59 to 400 of SEQ ID NO: 4 or an amino acid sequence that differs from amino acid 59 to 400 of SEQ ID NO: 4 by only having conservative substitutions. Or, the nucleic acid sequence encodes a modified MEK2 peptide having an amino acid sequence of amino acids 62 to 400 of SEQ ID NO: 4 or an amino acid sequence that differs from amino acid 62 to 400 of SEQ ID NO: 4 by only having conservative substitutions. Additionally, the nucleic acid sequence encodes a modified MEK2 peptide having an amino acid sequence of amino acids 64 to 400 of SEQ ID NO: 4 or an amino acid sequence that differs from amino acid 64 to 400 of SEQ ID NO: 4 by only having conservative substitutions. Such polynucleotides may be, for example, one having the sequence set forth in SEQ ID NO: 3 with deletion of the portion encoding the first 45-65 amino residues of the sequence of SEQ ID NO: 4.

[0098] Also, any of these amino acid sequences may contain one or more selenomethionines in place of a methionine. Further, these modified MEK2 peptides and their various variants may have a histidine oligomer tag, for example a histidine hexamer tag (His-tag) at their COOH-terminus.

[0099] As used herein, an "isolated" nucleic acid molecule is one that is separated from other nucleic acid present in the natural source of the nucleic acid. Preferably, an "isolated" nucleic acid is free of sequences which naturally flank the nucleic acid (i.e., sequences located at the 5' and 3' ends of the nucleic acid) in the genomic DNA or cDNA of the organism from which the nucleic acid is derived. However, there can be some flanking nucleotide sequences, for example up to about 5KB, particularly contiguous peptide encoding sequences and peptide encoding sequences within

the same gene but separated by introns in the genomic sequence. The important point is that the nucleic acid is isolated from remote and unimportant flanking sequences such that it can be subjected to the specific manipulations described herein such as recombinant expression, preparation of probes and primers, and other uses specific to the nucleic acid sequences.

[0100] Moreover, an "isolated" nucleic acid molecule, such as a cDNA molecule, can be substantially free of other cellular material, or culture medium when produced by recombinant techniques, or chemical precursors or other chemicals when chemically synthesized. However, the nucleic acid molecule can be fused to other coding or regulatory sequences and still be considered isolated.

[0101] For example, recombinant DNA molecules contained in a vector are considered isolated. Further examples of isolated DNA molecules include recombinant DNA molecules maintained in heterologous host cells or purified (partially or substantially) DNA molecules in solution. Isolated RNA molecules include *in vivo* or *in vitro* RNA transcripts of the isolated DNA molecules of the present invention. Isolated nucleic acid molecules according to the present invention further include such molecules produced synthetically.

[0102] The preferred classes of nucleic acid molecules that are comprised of the nucleotide sequences of the present are the full-length cDNA molecules and genes and genomic clones since some of the nucleic acid molecules provided in SEQ ID NO: 1 are fragments of the complete gene that exists in nature. A brief description of how various types of these nucleic acid molecules can be readily made/isolated is provided herein.

[0103] Full-length genes may be cloned from known sequence using any one of a number of methods known in the art. For example, a method which employs XL-PCR (Perkin-Elmer, Foster City, Calif.) to amplify long pieces of DNA may be used. Other methods for obtaining full-length sequences are known in the art.

[0104] The isolated nucleic acid molecules can encode the active protein plus additional amino or carboxyl-terminal amino acids, or amino acids interior to the mature peptide (when the mature form has more than one peptide chain, for instance). Such sequences may play a role in processing of a protein from precursor to an active form, facilitate protein trafficking, prolong or shorten protein half-life or facilitate manipulation of a protein for assay or production, among other things. As generally is the case *in situ,* the additional amino acids may be processed away from the mature active protein by cellular enzymes.

[0105] As mentioned above, the isolated nucleic acid molecules include, but are not limited to, the sequence encoding the active kinase alone or in combination with coding sequences, such as a leader or secretary sequence (e.g., a pre-pro or pro-protein sequence), the sequence encoding the active kinase, with or without the additional coding sequences, plus additional non-coding sequences, for example introns and non-coding 5' and 3' sequences such as transcribed but non-translated sequences that play a role in transcription, mRNA processing (including splicing and polyadenylation signals), ribosome binding and stability of mRNA. In addition, the nucleic acid molecule may be fused to a marker sequence encoding, for example, a peptide that facilitates purification.

[0106] Isolated nucleic acid molecules can be in the form of RNA, such as mRNA, or in the form of DNA, including cDNA and genomic DNA, obtained by cloning or produced by chemical synthetic techniques or by a combination thereof. The nucleic acid, especially DNA, can be double-stranded or single-stranded. Single-stranded nucleic acid can be the coding strand (sense strand) or the non-coding strand (antisense strand).

[0107] The invention further provides nucleic acid molecules that encode fragments of the peptides of the present invention and that encode obvious variants of the kinase proteins of the present invention that are described above. Such nucleic acid molecules may be naturally occurring, such as allelic variants (same locus), paralogs (different locus), and orthologs (different organism), or may be constructed by recombinant DNA methods or by chemical synthesis. Such non-naturally occurring variants may be made by mutagenesis techniques, including those applied to nucleic acid molecules, cells, or organisms. Accordingly, as discussed above, the variants can contain nucleotide substitutions, deletions, inversions and insertions. Variation can occur in either or both the coding and non-coding regions. The variations can produce both conservative and non-conservative amino acid substitutions.

[0108] A fragment comprises a contiguous nucleotide sequence greater than 12 or more nucleotides. Further, a fragment could be at least 30, 40, 50, 100, 250 or 500 nucleotides in length. The length of the fragment will be based on its intended use. For example, the fragment can encode epitope bearing regions of the peptide, or can be useful as DNA probes and primers. Such fragments can be isolated using the known nucleotide sequence to synthesize an oligonucleotide probe. A labeled probe can then be used to screen a cDNA library, genomic DNA library, or mRNA to isolate nucleic acid corresponding to the coding region. Further, primers can be used in PCR reactions to clone specific regions of gene.

[0109] A probe/primer typically comprises substantially a purified oligonucleotide or oligonucleotide pair. The oligonucleotide typically comprises a region of nucleotide sequence that hybridizes under stringent conditions to at least about 12, 20, 25, 40, 50 or more consecutive nucleotides.

[0110] Orthologs, homologs, and allelic variants can be identified using methods known in the art. As described above, these variants comprise a nucleotide sequence encoding a peptide that is typically 60%, preferably 65%, more preferably 70%, or even more preferably 75% or more homologous to the nucleotide sequence provided in SEQ ID

NO: 1 or SEQ ID NO: 3 or a fragment of this sequence. In one preferred embodiment, the variants comprise a nucleotide sequence encoding a peptide that is at least 80%, preferably 85%, more preferably 90%, even more preferably 95% or more homologous to the nucleotide sequence provided in SEQ ID NO: 1 or SEQ ID NO: 3 or a fragment of this sequence. Such nucleic acid molecules can readily be identified as being able to hybridize under moderate to stringent conditions, to the nucleotide sequence shown in SEQ ID NO: 1 or SEQ ID NO: 3 or a fragment of the sequence.

[0111] As used herein, the term "hybridizes under stringent conditions" is intended to describe conditions for hybridization and washing under which nucleotide sequences encoding a peptide at least 50%, preferably at least 55% homologous to each other typically remain hybridized to each other. The conditions can be such that sequences at least 65%, preferably at least 70%, or more preferably at least 75% homologous to each other typically remains hybridized to each other. Standard hybridization conditions from moderate to highly stringent conditions are known to those skilled in the art (See e.g., *Current Protocols in Molecular Biology,* John Wiley & Sons, N.Y. (1989), 6.3.1-6.3.6). Moderate hybridization conditions are defined as equivalent to hybridization in 2X sodium chloride/sodium citrate (SSC) at 30 °C, followed by one or more washes in 1X SSC, 0.1% SDS at 50-60 °C. Highly stringent conditions are defined as equivalent to hybridization in 6X sodium chloride/sodium citrate (SSC) at 45 °C, followed by one or more washes in 0.2X SSC, 0.1% SDS at 50-65 °C.

[0112] The nucleic acid molecules of the present invention are useful for probes, primers, chemical intermediates, and in biological assays. The nucleic acid molecules are useful as a hybridization probe for cDNA and genomic DNA to isolate full-length cDNA and genomic clones encoding the peptide described herein and to isolate cDNA and genomic clones that correspond to variants (alleles, orthologs, etc.) producing the same or related peptides described herein.

[0113] The probe can correspond to any sequence along the entire length of the nucleic acid molecules provided in the SEQ ID NO: 1 or SEQ ID NO: 3. Accordingly, it could be derived from 5' noncoding regions, the coding region, and 3' noncoding regions. However, as discussed, fragments are not to be construed as those which may encompass fragments disclosed prior to the present invention.

[0114] The nucleic acid molecules are also useful as primers for PCR to amplify any given region of a nucleic acid molecule and are useful to synthesize antisense molecules of desired length and sequence.

[0115] The nucleic acid molecules are also useful for constructing recombinant vectors. Such vectors include expression vectors that express a portion of, or all of, the peptide sequences. Vectors also include insertion vectors, used to integrate into another nucleic acid molecule sequence, such as into the cellular genome, to alter *in situ* expression of a gene and/or gene product. For example, an endogenous coding sequence can be replaced via homologous recombination with all or part of the coding region containing one or more specifically introduced mutations. The nucleic acid molecules are also useful for expressing antigenic portions of the proteins; useful as probes for determining the chromosomal positions of the nucleic acid molecules by means of *in situ* hybridization methods; useful for designing ribozymes corresponding to all, or a part, of the mRNA produced from the nucleic acid molecules described herein; and useful for constructing host cells expressing a part, or all, of the nucleic acid molecules and peptides. The nucleic acid molecules are also useful for constructing transgenic animals expressing all, or a part, of the nucleic acid molecules and peptides; and useful for making vectors that express part, or all, of the peptides. The nucleic acid molecules are further useful as hybridization probes for determining the presence, level, form and distribution of nucleic acid expression. Accordingly, the probes can be used to detect the presence of, or to determine levels of, a specific nucleic acid molecule in cells, tissues, and in organisms. The nucleic acid whose level is determined can be DNA or RNA. Accordingly, probes corresponding to the peptides described herein can be used to assess expression and/or gene copy number in a given cell, tissue, or organism. These uses are relevant for diagnosis of disorders involving an increase or decrease in kinase protein expression relative to normal results.

[0116] *In vitro* techniques for detection of mRNA include Northern hybridizations and *in situ* hybridizations. *In vitro* techniques for detecting DNA includes Southern hybridizations and *in situ* hybridization.

[0117] Probes can be used as a part of a diagnostic test kit for identifying cells or tissues that express a kinase protein, such as by measuring a level of a receptor-encoding nucleic acid in a sample of cells from a subject e.g., mRNA or genomic DNA, or determining if a receptor gene has been mutated.

Vectors And Host Cells For Producing Modified MEK1 and MEK2 Peptides

[0118] The present invention also provides for an expression vector for producing the modified MEK1 and MEK2 peptides described above in a host cell. It further provides a host cell which may be stably transformed and transfected with a polynucleotide encoding the modified MEK1 and MEK2 peptides described above, or a fragment thereof or an analog thereof, in a manner allowing the expression of the modified MEK1 and MEK2 peptides. The present invention also provides expression vectors comprising the nucleic acids of the present invention operatively associated with an expression control sequence.

MEK1 Expresion Vectors

[0119] The expression vector may contain a nucleic acid encoding a modified MEK1 peptide having an amino acid sequence from between amino acids 42 and 62 to amino acid 393 of SEQ ID NO: 2 or a conservatively substituted variant thereof. In one embodiment, the expression vector contains a nucleic acid encoding a modified MEK1 peptide having an amino acid sequence of amino acids 42 to 393 of SEQ ID NO: 2 or an amino acid sequence that differs from amino acid 42 to 393 of SEQ ID NO: 2 by only having conservative substitutions. In an alternative embodiment, the expression vector contains a nucleic acid encoding a modified MEK1 peptide having an amino acid sequence between amino acids 51 to 393 of SEQ ID NO: 2 or an amino acid sequence that differs from amino acids 51 to 393 of SEQ ID NO: 2 by only having conservative substitutions. In still another embodiment, the expression vector contains a nucleic acid encoding a NH_2-terminally truncated MEK1 peptide having an amino acid sequence of amino acids 62 to 393 of SEQ ID NO: 2 or an amino acid sequence that differs from amino acids 62 to 393 of SEQ ID NO: 2 by only having conservative substitutions. Such polynucleotides may be, for example, one having the sequence set forth in SEQ ID NO: 1 with deletion of the portion encoding the first 41 - 61 amino residues of the sequence of SEQ ID NO: 2.

[0120] In addition, the expression vector may contain a nucleic acid encoding a modified MEK1 having a NH_2-terminal truncation and a deletion of insertion loop-forming amino acid residues, particularly from amino acid 280 to amino acid 323 SEQ ID NO: 2; or at least 40 amino acids from between amino acid residue 264 and amino acid 310 of SEQ ID NO: 2. This may include a deletion of amino acids (1) from amino acid 264 to amino acid 310 of SEQ ID NO: 2; (2) from amino acid 270 to amino acid 310 of SEQ ID NO: 2; (3) from amino acid 264 to amino acid 305 of SEQ ID NO: 2; (4) amino acid 267 to amino acid 307 of SEQ ID NO: 2; or (5) from amino acid 265 to amino acid 304 of SEQ ID NO: 2. Further, such polynucleotide may encode the MEK1 peptide modified to have a deletion of insertion loop-forming amino acid residues as described above without NH_2-terminal truncation.

[0121] Also, the expression vector may contain a nucleic acid encoding a modified MEK1 peptide wherein the insertion loop-forming amino acid residues are replaced with a linker peptide, preferably Lys-Asn-Cys-Lys-Thr-Asp, with or without NH_2-terminal truncation as described above.

[0122] Also, any of these expression vectors may optionally contain a nucleic acid encoding a modified MEK1 peptide having one or more selenomethionines in place of a methionine. The expression vector may also optionally contain a nucleic acid encoding a modified MEK1 peptide having a histidine oligomer tag, for example a histidine hexamer tag (His-tag) at its COOH-terminus.

MEK2 Expresion Vectors

[0123] The expression vectors of the invention may also contain a nucleic acid encoding a modified MEK2 peptide having an amino acid sequence from between amino acids 46 and 66 to amino acid 400 of SEQ ID NO: 4 or a conservatively substituted variant thereof. In particular, the expression vector may contain a nucleic acid sequence encoding a modified MEK2 peptide having an amino acid sequence of amino acids 46 to 400 of SEQ ID NO: 4 or an amino acid sequence that differs from amino acid 46 to 400 of SEQ ID NO: 4 by only having conservative substitutions. Alternatively, the expression vector may contain a nucleic acid sequence encoding a modified MEK2 peptide having an amino acid sequence of amino acids 55 to 400 of SEQ ID NO: 4 or an amino acid sequence that differs from amino acid 55 to 400 of SEQ ID NO: 4 by only having conservative substitutions. Or, the expression vector may contain a nucleic acid sequence encoding a modified MEK2 peptide having an amino acid sequence of amino acids 66 to 400 of SEQ ID NO: 4 or an amino acid sequence that differs from amino acid 66 to 400 of SEQ ID NO: 4 by only having conservative substitutions. Alternatively, the expression vector may contain a nucleic acid sequence encoding a modified MEK2 peptide having an amino acid sequence of amino acids 59 to 400 of SEQ ID NO: 4 or an amino acid sequence that differs from amino acid 59 to 400 of SEQ ID NO: 4 by only having conservative substitutions. Or, the expression vector may contain a nucleic acid sequence encoding a modified MEK2 peptide having an amino acid sequence of amino acids 62 to 400 of SEQ ID NO: 4 or an amino acid sequence that differs from amino acid 62 to 400 of SEQ ID NO: 4 by only having conservative substitutions. Additionally, the expression vector may contain a nucleic acid sequence encoding a modified MEK2 peptide having an amino acid sequence of amino acids 64 to 400 of SEQ ID NO: 4 or an amino acid sequence that differs from amino acid 64 to 400 of SEQ ID NO: 4 by only having conservative substitutions. Such expression vectors may be, for example, one containing a nucleic acid sequence encoding the sequence set forth in SEQ ID NO: 3 with deletion of the portion encoding the first 45-65 amino residues of the sequence of SEQ ID NO: 4.

[0124] Also, any of these expression vectors may optionally contain a nucleic acid encoding a modified MEK2 peptide having one or more selenomethionines in place of a methionine. The expression vector may also optionally contain a nucleic acid encoding a modified MEK2 peptide having a histidine oligomer tag, for example a histidine hexamer tag (His-tag) at its COOH-terminus.

[0125] The present invention further includes a cell transfected or transformed with an expression vector of the

present invention. Any of the cells mentioned below may be employed in this method. In one embodiment, the cell is a prokaryotic cell. Preferably, the prokaryotic cell is an *E. coli* cell. In another embodiment the cell is an eukaryotic cell, such as an insect cell or a vertebrate cell, which may be, for example, a mammalian cell.

[0126] The present invention also includes methods for expressing the modified MEK1 and MEK2 peptides comprising culturing a cell that expresses the modified MEK1 or MEK2 peptide in an appropriate cell culture medium under conditions that provide for expression of the protein by the cell. Any of the cells mentioned above may be employed in this method. In a particular embodiment, the cell is a yeast cell which has been manipulated to express a modified MEK1 or MEK2 peptide of the present invention. In a preferred embodiment, the prokaryotic cell is an *E. coli* cell which has been manipulated to express a modified MEK1 or MEK2 peptide of the present invention.

[0127] The invention also provides vectors containing the nucleic acid molecules described herein. The term "vector" refers to a vehicle, preferably a nucleic acid molecule that can transport the nucleic acid molecules. When the vector is a nucleic acid molecule, the nucleic acid molecules are covalently linked to the vector nucleic acid. The vector preferably includes a plasmid, single or double stranded phage, a single or double stranded RNA or DNA viral vector, or artificial chromosome, such as aBAC, PAC, YAC, or MAC, which are commercially available from, for example, Qiagen (Valencia, CA). Various expression vectors known in the art can be used to express polynucleotide encoding the MEK1 or MEK2 peptide.

[0128] A vector can be maintained in the host cell as an extrachromosomal element where it replicates and produces additional copies of the nucleic acid molecules. Alternatively, the vector may integrate into the host cell genome and produce additional copies of the nucleic acid molecules when the host cell replicates.

[0129] The invention provides vectors for the maintenance (cloning vectors) or vectors for expression (expression vectors) of the nucleic acid molecules. The vectors can function in prokaryotic or eukaryotic cells or in both (shuttle vectors).

[0130] Expression vectors contain cis-acting regulatory regions that are operably linked in the vector to the nucleic acid molecules such that transcription of the nucleic acid molecules is allowed in a host cell. The nucleic acid molecules can be introduced into the host cell with a separate nucleic acid molecule capable of affecting transcription. Thus, the second nucleic acid molecule may provide a trans-acting factor interacting with the cis-regulatory control region to allow transcription of the nucleic acid molecules from the vector. Alternatively, a trans-acting factor may be supplied by the host cell. Finally, a trans-acting factor can be produced from the vector itself. It is understood, however, that in some embodiments, transcription and/or translation of the nucleic acid molecules can occur in a cell-free system.

[0131] The regulatory sequence to which the nucleic acid molecules described herein can be operably linked include promoters for directing mRNA transcription. These include, but are not limited to, the left promoter from bacteriophage λ, the lac, TRP, and TAC promoters from *E. coli,* the early and late promoters from SV40, the CMV immediate early promoter, the adenovirus early and late promoters, and retrovirus long-terminal repeats.

[0132] In addition to control regions that promote transcription, expression vectors may also include regions that modulate transcription, such as repressor binding sites and enhancers. Examples include the SV40 enhancer, the cytomegalovirus immediate early enhancer, polyoma enhancer, adenovirus enhancers, and retrovirus LTR enhancers.

[0133] In addition to containing sites for transcription initiation and control, expression vectors can also contain sequences necessary for transcription termination and, in the transcribed region a ribosome-binding site for translation. Other regulatory control elements for expression include initiation and termination codons as well as polyadenylation signals. The person of ordinary skill in the art would be aware of the numerous regulatory sequences that are useful in expression vectors. Such regulatory sequences are described, for example, in Sambrook *et al., (Molecular Cloning: A Laboratory Manual. 2nd. ed.,* Cold Spring Harbor Laboratory Press, Cold Spring Harbor, NY, (1989)).

[0134] A variety of expression vectors can be used to express a nucleic acid molecule. Such vectors include chromosomal, episomal, and virus-derived vectors, for example vectors derived from bacterial plasmids, from bacteriophage, from yeast episomes, from yeast chromosomal elements, including yeast artificial chromosomes, from viruses such as baculoviruses, papovaviruses such as SV40, Vaccinia viruses, adenoviruses, poxviruses, pseudorabies viruses, and retroviruses. Vectors may also be derived from combinations of these sources such as those derived from plasmid and bacteriophage genetic elements, e.g., cosmids and phagemids. Appropriate cloning and expression vectors for prokaryotic and eukaryotic hosts are described in Sambrook *et al., Molecular Cloning: A Laboratory Manual. 2nd. ed.,* Cold Spring Harbor Laboratory Press, Cold Spring Harbor, NY, (1989).

[0135] The regulatory sequence may provide constitutive expression in one or more host cells (i.e. tissue specific) or may provide for inducible expression in one or more cell types such as by temperature, nutrient additive, or exogenous factor such as a hormone or other ligand. A variety of vectors providing for constitutive and inducible expression in prokaryotic and eukaryotic hosts are known to those of ordinary skill in the art.

[0136] The nucleic acid molecules can be inserted into the vector nucleic acid by well-known methodology. Generally, the DNA sequence that will ultimately be expressed is joined to an expression vector by cleaving the DNA sequence and the expression vector with one or more restriction enzymes and then ligating the fragments together. Procedures for restriction enzyme digestion and ligation are known to those of ordinary skill in the art.

[0137] The vector containing the appropriate nucleic acid molecule can be introduced into an appropriate host cell for propagation or expression using well-known techniques. Bacterial cells include, but are not limited to, *E. coli, Streptomyces*, and *Salmonella typhimurium.* Eukaryotic cells include, but are not limited to, yeast, insect cells such as *Drosophila*, animal cells such as COS and CHO cells, and plant cells.

[0138] As described herein, it may be desirable to express a peptide of the present invention as a fusion protein. Accordingly, the invention provides fusion vectors that allow for the production of such peptides. Fusion vectors can increase the expression of a recombinant protein, increase the solubility of the recombinant protein, and aid in the purification of the protein by acting for example as a ligand for affinity purification. A proteolytic cleavage site may be introduced at the junction of the fusion moiety so that the desired peptide can ultimately be separated from the fusion moiety. Proteolytic enzymes include, but are not limited to, factor Xa, thrombin, and enterokinase. Typical fusion expression vectors include pRS (Sikorski, et al., *Genetics* 122(1): 19-27 (1989)), pGEX (Smith *et al., Gene 67:* 31-40 (1988)), pMAL (New England Biolabs, Beverly, MA) and pRIT5 (Pharmacia, Piscataway, NJ) which fuse glutathione S-transferase (GST), maltose E binding protein, or protein A, respectively, to the target recombinant protein. Examples of suitable inducible non-fusion *E. coli* expression vectors include pTrc (Amann *et al., Gene 69*: 301-315 (1988)) and pET 11d (Studier *et al., Gene Expression Technology: Methods in Enzymology* 185: 60-89 (1990)).

[0139] Recombinant protein expression can be maximized in a host bacteria by providing a genetic background wherein the host cell has an impaired capacity to proteolytically cleave the recombinant protein. (Gottesman, S., *Gene Expression Technology: Methods in Enzymology* 185, Academic Press, San Diego, California 119-128 (1990)). Alternatively, the sequence of the nucleic acid molecule of interest can be altered to provide preferential codon usage for a specific host cell, for example *E. coli.* (Wada *et al., Nucleic Acids Res. 20*: 2111-2118 (1992)).

[0140] The nucleic acid molecules can also be expressed by expression vectors that are operative in yeast. Examples of vectors for expression in yeast e.g., *S. cerevisiae* include pYepSec1 (Baldari, *et al., EMBO J. 6*: 229-234 (1987)), pMFa (Kurjan *et al., Cell 30:* 933-943 (1982)), pJRY88 (Schultz *et al., Gene 54*: 113-123 (1987)), and pYES2 (Invitrogen Corporation, San Diego, CA).

[0141] The nucleic acid molecules can also be expressed in insect cells using, for example, baculovirus expression vectors. Baculovirus vectors available for expression of proteins in cultured insect cells (e.g., Sf9 cells) include the pAc series (Smith *et al., Mol. Cell Biol. 3:* 2156-2165 (1983)) and the pVL series (Lucklow *et al., Virology 170:* 31-39 (1989)). In certain embodiments of the invention, the nucleic acid molecules described herein are expressed in mammalian cells using mammalian expression vectors. Examples of mammalian expression vectors include pCDM8 (Seed, B. *Nature 329:* 840 (1987)) and pMT2PC (Kaufman *et al., EMBO J. 6*: 187-195 (1987)).

[0142] The expression vectors listed herein are provided by way of example only of the well-known vectors available to those of ordinary skill in the art that would be useful to express the nucleic acid molecules. Preferred vectors include the pET24b (Novagen, Madison, WI), pAcSG2 (Pharmingen, San Diego, CA), and pFastBac (Life Technologies, Gaithersburg, MD). The person of ordinary skill in the art would be aware of other vectors suitable for maintenance propagation or expression of the nucleic acid molecules described herein. These are found for example in Sambrook, J., Fritsh, E. F., and Maniatis, T. *Molecular Cloning: A Laboratory Manual. 2nd, ed., Cold Spring Harbor Laboratory*, Cold Spring Harbor Laboratory Press, Cold Spring Harbor, NY, 1989.

[0143] The invention also encompasses vectors in which the nucleic acid sequences described herein are cloned into the vector in reverse orientation, but operably linked to a regulatory sequence that permits transcription of antisense RNA. Thus, an antisense transcript can be produced to all, or to a portion, of the nucleic acid molecule sequences described herein, including both coding and non-coding regions. Expression of this antisense RNA is subject to each of the parameters described above in relation to expression of the sense RNA (regulatory sequences, constitutive or inducible expression, tissue-specific expression).

[0144] The invention also relates to recombinant host cells containing the vectors described herein. Host cells therefore include, for example, prokaryotic cells, lower eukaryotic cells such as yeast, other eukaryotic cells such as insect cells, and higher eukaryotic cells such as mammalian cells. Preferred host cells of the instant invention include *E. coli* and Sf9.

[0145] The recombinant host cells are prepared by introducing the vector constructs described herein into the cells by techniques readily available to the person of ordinary skill in the art. These include, but are not limited to, calcium phosphate transfection, DEAE-dextran-mediated transfection, cationic lipid-mediated transfection, electroporation, transduction, infection, lipofection, and other techniques such as those found in Sambrook, *et al.* (*Molecular Cloning: A Laboratory Manual. 2nd, ed., Cold Spring Harbor Laboratory*, Cold Spring Harbor Laboratory Press, Cold Spring Harbor, NY, 1989).

[0146] Host cells can contain more than one vector. Thus, different nucleotide sequences can be introduced on different vectors of the same cell. Similarly, the nucleic acid molecules can be introduced either alone or with other nucleic acid molecules that are not related to the nucleic acid molecules such as those providing trans-acting factors for expression vectors. When more than one vector is introduced into a cell, the vectors can be introduced independently, co-introduced or joined to the nucleic acid molecule vector.

[0147] In the case of bacteriophage and viral vectors, these can be introduced into cells as packaged or encapsulated virus by standard procedures for infection and transduction. Viral vectors can be replication-competent or replication-defective. In the case in which viral replication is defective, replication will occur in host cells providing functions that complement the defects.

[0148] Vectors generally include selectable markers that enable the selection of the subpopulation of cells that contain the recombinant vector constructs. The marker can be contained in the same vector that contains the nucleic acid molecules described herein or may be on a separate vector. Markers include tetracycline or ampicillin-resistance genes for prokaryotic host cells and dihydrofolate reductase or neomycin resistance for eukaryotic host cells. However, any marker that provides selection for a phenotypic trait will be effective.

[0149] While the active protein kinases can be produced in bacteria, yeast, mammalian cells, and other cells under the control of the appropriate regulatory sequences, cell- free transcription and translation systems can also be used to produce these proteins using RNA derived from the DNA constructs described herein.

[0150] Where secretion of the peptide is desired, appropriate secretion signals are incorporated into the vector. The signal sequence can be endogenous to the proteins or heterologous to these proteins.

[0151] It is also understood that depending upon the host cell in recombinant production of the peptides described herein, the peptides can have various glycosylation patterns, depending upon the cell, or maybe non-glycosylated as when produced in bacteria. In addition, the peptides may include an initial modified methionine in some cases as a result of a host-mediated process.

[0152] The recombinant host cells expressing the peptides described herein have a variety of uses. First, the cells are useful for producing the MEK1 and MEK2 peptides or a peptide that can be further purified to produce desired amounts of the peptide or fragments. Thus, host cells containing expression vectors are useful for peptide production.

[0153] Host cells are also useful for conducting cell-based assays involving the protein or protein fragments. Thus, a recombinant host cell expressing a native protein is useful for assaying compounds that stimulate or inhibit protein function.

[0154] Host cells are also useful for identifying protein mutants in which these functions are affected. If the mutants naturally occur and give rise to a pathology, host cells containing the mutations are useful to assay compounds that have a desired effect on the mutant protein (for example, stimulating or inhibiting function) which may not be indicated by their effect on the native protein.

[0155] Genetically engineered host cells can be further used to produce non-human transgenic animals. A transgenic animal is preferably a mammal, for example a rodent, such as a rat or mouse, in which one or more of the cells of the animal include a transgene. A transgene is exogenous DNA which is integrated into the genome of a cell from which a transgenic animal develops and which remains in the genome of the mature animal in one or more cell types or tissues of the transgenic animal. These animals are useful for studying the function of the MEK1 or MEK2 peptide and identifying and evaluating modulators of the protein activity. Other examples of transgenic animals include non-human primates, sheep, dogs, cows, goats, chickens, and amphibians.

Peptide Purification of Modified MEK1 and MEK2

[0156] The purification conditions and methods listed herein are provided to elucidate the approach used in the purification of the MEK1 and MEK2 peptides and for the formation, for example, of the MEK1: ligand: cofactor and MEK2:ligand:cofactor complexes. Of course those of ordinary skill in the art would be aware of other purification conditions and techniques that may be suitable for the purification of the modified MEK1 and MEK2 proteins described herein. For examples see, Methods in Enzymology, Volume 182; Guide to Protein Purification, edited by M.P. Duetscher; Academic Press (1990).

Purification of Modified MEK1

[0157] The invention provides a multiple step method for purifying the modified MEK1 peptide, described herein, to near homogeneity. The modified MEK1 peptide, preferably the MEK1 peptide with a poly-histidine tag at the COOH-terminus, may be advantageously purified by employing immobilized metal affinity chromatography (IMAC). The immobilized metal may be nickel, zinc, cobalt, or copper. Preferably, the immobilized metal is cobalt, as found in the TALON™ metal affinity resin from ClonTech. The IMAC step may be performed on the soluble fraction of the fermentation broth containing the expressed MEK1 peptide, which is obtained after the host cell lysis. The host cell lysis processes are known to those skilled in the art and may be selected for by them without difficulty. For example, when *E. coli* is used as host cell for expressing the MEK1 peptides, *E. coli* cell lysis may be enzymatically performed, for example by using lysozyme. Alternatively, mechanical processes using a french press, sonicator, or bead bill may be employed. Preferably, a mechanical lysis using a bead mill (DynoMill KDL) is used to perform *E. coli* cell lysis.

[0158] The modified MEK1 peptide, preferably the MEK1 peptide containing the COOH-terminal His-Tag, may be

purified by immobilized metal chelate (IMAC) chromatography. The IMAC step may be accomplished with the following resins, but not limited to: Ni-NTA™ resin from Qiagen, HisTrap™ resin from Pharmacia, POROS™ MC resin from Applied Biosystems or TALON resin from Clontech. Preferably, TALON resin is used. More preferably, the IMAC step is accomplished by the use of resin in a ratio of about 2 mL resin to about 1 g wet weight of whole cells, prior to cell lysis.

[0159] An additional aspect of the invention includes the use of a transition state analogue and a metal cation to displace a contaminant protein during the IMAC purification. When *E. coli* is employed as a host cell for expressing the MEK1 peptides, contaminant proteins such as *E. coli* prolyl isomerase are contained in the fermentation broth, and are preferably removed before crystallization. For the invention, a transition state analogue and a metal cation are employed to replace the contaminant protein during MEK1-binding and contaminant removal steps of the IMAC purification. The transition state analogue may be, but is not limited to, pyrrole-2-carboxylate, Δ-1-pyrroline-2-carboxylate, or tetrahydrofuran-2-carboxylate. Preferably, the transition state analogue is pyrrole-2-carboxylate. The transition state analogue, if present, has a concentration of from about 0.1 mM to about 20.0 mM, and even more preferably has a concentration of about 1.0 mM. As a source of the metal cation, a form of the zinc cation may be employed. It may be used in any salt form, for example zinc acetate, zinc chloride or zinc sulfate. Preferably, zinc is used in the form of zinc chloride at a concentration of about 0.05 mM.

[0160] The MEK1-binding and contaminant removal steps of the IMAC purification may be performed in the presence of any suitable buffering agent. For example, the buffering agent may be, but is not limited to, Tris [Tris(hydroxymethyl)-aminomethane], HEPES (N-2-hydroxyethyl-piperazine-N'-2-ethanesulfonic acid), potassium phosphate, citrate-phosphate, sodium phosphate, ammonium monobasic phosphate, or MOPS (3-(N-morpholino) propanesulfonic acid). Preferably, the buffering agent is about 50.0 mM ammonium or potassium monobasic phosphate having a pH of about 8.0.

[0161] The binding and contaminant removal steps of the IMAC purification may be performed in the presence of any suitable contaminating protein-displacing agents. The contaminating protein-displacing agent may be, but is not limited to, imidazole, or histidine. Preferably, the contaminating protein-displacing agent is about 5.0 mM imidazole.

[0162] The binding and contaminant removal steps of the IMAC purification can be performed in the presence of any suitable reducing agents. The reducing agent may be, but is not limited to, 2-mercaptoethanol, or TCEP (Tris[2-Carboxyethylphosphine] hydrochloride). Preferably, the reducing agent is about 2.0 mM TCEP.

[0163] The binding and contaminant removal steps of the IMAC purification may be performed in the presence of a detergent. The detergent may be, but is not limited to, CHAPS (3-([3-cholamidopropyl]-dimethylammonio)-1-propanesulfonate), Triton X-100, Nonidet P-40, Tween 20, or Tween 80. Preferably, the detergent is about 10.0 mM CHAPS.

[0164] The binding and contaminant removal steps of the IMAC purification may be performed in the presence of an ion source. The ion source may be, but is not limited to, KCl, NaCl, or sodium sulfate. Preferably, an ion source is about 0.3 M NaCl.

[0165] The elution of MEK1 from the IMAC resin may be accomplished by several modes, which are known in the art. For example, the elution of MEK1 from the IMAC column may be accomplished by using, for example, EDTA, histidine, or imidazole, or by reducing the pH. Preferably, the elution of MEK1 may be accomplished with about 100 mM EDTA.

[0166] The elution step of the IMAC purification may be performed in the presence of any suitable buffering agent (s). The buffering agent may be, but is not limited to, Tris, ammonium monobasic phosphate, HEPES, or MOPS. Preferably, the buffering agent may be about 20.0 mM HEPES or (pH of about 8.0). The elution of MEK1 also may be performed in the presence of any suitable organic agents. The organic agent may be, but is not limited to, glycerol or ethylene glycol. Preferably, the organic agent is about 10% glycerol.

[0167] The invention also provides a method for further purifying the protein using cation and anion exchange chromatography, followed by size exclusion chromatography (SEC). The cation exchange chromatography could occur prior to the anion exchange chromatography, or alternatively, the anion exchange chromatography could occur prior to the cation exchange chromatography. Further, the ion exchange steps could be eliminated all together. The preferred method is to perform the cation exchange step prior to the anion exchange step, which is followed by protein concentration and size exclusion chromatography.

[0168] The cation exchange step may be performed using several types of chromatography resins. For example, the cation exchange resin may be, but is not limited to, S-Sepharose™, MonoS™, POROS™ HS, or POROS™ S. Preferably, the cation exchange resin is POROS™ HS. The cation exchange step may be performed in the presence of any suitable buffering agent(s). The buffering agent may include, but is not limited to, phosphate, malonic acid, butanedioic acid, acetic acid, MES (2-(N-morpholino)-ethanesulfonic acid), or HEPES. Preferably, the buffering agent is about 20.0 mM MES (pH of about 6.4).

[0169] The cation exchange step may be performed in the presence of any suitable reducing agent(s). The reducing agent may be, but is not limited to, 2-mercaptoethanol, TCEP, or dithiothreitol (DTT). Preferably, the reducing agent is about 2.0 mM TCEP.

[0170] The cation exchange step may be performed in the presence of any suitable organic agent(s). The organic

agent may be, but is not limited to, glycerol or ethylene glycol. Preferably, the organic agent is about 20.0% ethylene glycol.

[0171] Elution of the MEK1 from the cation exchange resin may be accomplished by several different modes that are known in the art. For example, the MEK1 may be eluted by increasing the pH. Alternatively, the MEK1 may be eluted by increasing the salt concentration by using, for example, NaC1, KC1, ammonium acetate, or sodium sulfate. Preferably, ammonium acetate may be used to cause the elution by an increase of the salt concentration.

[0172] The anion exchange step may be performed using several types of chromatography resin(s). The anion exchange resin may be, but is not limited to, Q-Sepharose™, DEAE-Sepharose™, MonoQ™, POROS™ HQ, or POROS™ PI. Preferably, the exchange resin is POROS™ HQ.

[0173] The anion exchange step may be performed in the presence of any suitable buffering agent(s). The buffering agent may be, but is not limited to, HEPES, Tris, bis-Tris, bis-Tris Propane, N-methyldiethanolamine, 1,3-diaminopropane, ethanolamine, piperazine, or ammonium monobasic phosphate. Preferably, the buffering agent is about 20.0 mM Tris (pH of about 8.0).

[0174] The anion exchange step may be performed in the presence of any suitable reducing agent(s). The reducing agent may be, but is not limited to, 2-mercaptoethanol, TCEP, or DTT. Preferably, the reducing agent is about 2.0 mM TCEP.

[0175] The anion exchange step may be performed in the presence of any suitable salt(s). The salt may be NaCl, KCl, ammonium acetate, or sodium sulfate. Preferably, the salt is about 10.0 mM ammonium acetate.

[0176] The SEC step may be performed using various types of chromatography resins. For example, the suitable SEC resin may include, but is not limited to, Sephadex™ G-100, Sephadex™ G-200, Sephacryl™ S-100, Sephacryl™ S-200, Superdex™ 75, or Superdex™ 200. Preferably, the SEC resin is Superdex™ 200.

[0177] The SEC step may performed in the presence of any suitable buffering agent(s). The buffering agent may be, but is not limited to, phosphate, HEPES, MES, Tris, bis-Tris, or bis-Tris propane. Preferably, the buffering agent is about 20.0 mM HEPES (pH of about 7.5).

[0178] The SEC step may be performed in the presence of any suitable reducing agent(s). The reducing agent may be, but is not limited to, 2-mercaptoethanol, TCEP, or DTT. Preferably, the reducing agent is about 2.0 mM TCEP.

[0179] The SEC step may be performed in the presence of any suitable salt(s). The salt may be, but is not limited to, NaCl, KCl, ammonium acetate, or sodium sulfate. Preferably, the salt is about 150.0 mM ammonium acetate.

[0180] The SEC step may be performed in the presence of any suitable chelating agent(s). The chelating agent may be, but is not limited to, sodium citrate or EDTA. Preferably, the salt is about 0.5 mM EDTA.

[0181] The invention also provides a method for forming a MEK1: ligand complex. The MEK1: ligand complex formation may be performed at any point during the MEK1 purification. Preferably, the MEK1: ligand complex formation step may be performed prior to the SEC step. Alternatively, the MEK1: ligand complex formation step could be performed after the protein has been completely purified. The MEK1: ligand complex formation step may be performed at various concentrations of MEK1. For example, the concentration of MEK1 may be in the range of about 0.02 mg/ml to about 2 mg/ml. Preferably, the concentration of MEK1 is about 0.2 mg/ml to about 0.3 mg/ml. Further, the MEK1: ligand complex formation step may be performed at various molar ratios of MEK1 to ligand. For example, the molar ratio of MEK1 to ligand may be in the range of about 1:1 to about 1:1000. Preferably, the molar ratio of MEK1 to ligand is about 1:10.

Purification of Modified MEK2

[0182] The invention also provides a multiple step method for purifying the modified MEK2 peptide, described herein, to near homogeneity. The modified MEK2 peptide, preferably the MEK2 peptide with a poly-histidine tag at the COOH-terminus, may be advantageously purified by employing immobilized metal affinity chromatography (IMAC). The immobilized metal may be, for example, nickel, zinc, cobalt, or copper. Preferably, the immobilized metal is cobalt, as found in the TALON™ metal affinity resin from ClonTech. The IMAC step may be performed on the soluble fraction of the fermentation broth containing the expressed MEK2 peptide, which is obtained after the host cell lysis. The host cell lysis processes are known to those skilled in the art and may be selected for by them without difficulty. For example, when *E. coli* is used as host cell for expressing the MEK2 peptides, *E. coli* cell lysis may be enzymatically performed, for example by using lysozyme. Alternatively, mechanical processes using a french press, sonicator, or bead bill may be employed. Preferably, a mechanical lysis using a bead mill (DynoMill KDL) is used to perform *E. coli* cell lysis.

[0183] The modified MEK2 peptide, preferably the MEK2 peptide containing the COOH-terminal His-Tag, may be purified by immobilized metal chelate (IMAC) chromatography. The IMAC step may be accomplished with, for example, the following resins: Ni-NTA™ resin from Qiagen, HisTrap™ resin from Pharmacia, POROS™ MC resin from Applied Biosystems or TALON resin from Clontech. Preferably, TALON resin is used. More preferably, the IMAC step is accomplished by the use of resin in a ratio of about 1 mL resin to about 5 g wet weight of whole cells, prior to cell lysis.

[0184] An additional aspect of the invention includes the use of a transition state analogue and metal to displace a

contaminant protein during the IMAC purification. When *E. coli* is employed as a host cell for expressing the MEK2 peptides, contaminant proteins such as *E. coli* prolyl isomerase are contained in the fermentation broth, and are preferably removed before crystallization. For the invention, a transition state analogue and a divalent metal cation are employed to displace the contaminant protein during the MEK2-binding and contaminant removal steps of the IMAC purification. The transition state analogue may be, but is not limited to, pyrrole-2-carboxylate, Δ-1-pyrroline-2-carboxylate, or tetrahydrofuran-2-carboxylate. Preferably, the transition state analogue is pyrrole-2-carboxylate. The transition state analogue, if present, has a concentration of from about 0.1 mM to about 20.0 mM, and even more preferably has a concentration of about 1.0 mM. As the divalent metal cation, zinc may be employed. It may be used in any salt form, for example zinc acetate, zinc chloride or zinc sulfate. Preferably, zinc is used in the form of zinc chloride at a concentration of about 0.05 mM.

[0185] The MEK2-binding and contaminant removal steps of the IMAC purification may be performed in the presence of any suitable buffering agent. For example, the buffering agent may be, but is not limited to, Tris [Tris(hydroxymethyl)-aminomethane], HEPES (N-2-hydroxyethyl-piperazine-N'-2-ethanesulfonic acid), potassium phosphate, citrate-phosphate, sodium phosphate, or MOPS (3-(N-morpholino) propanesulfonic acid). Preferably, buffering agent is about 50.0 mM potassium phosphate having pH of about 8.0.

[0186] The binding and contaminant removal steps of the IMAC purification may be performed in the presence of any suitable contaminating protein-displacing agents. The contaminating protein-displacing agent may be, but is not limited to, imidazole, or histidine. Preferably, the contaminating protein-displacing agent is about 5.0 mM imidazole.

[0187] The binding and contaminant removal steps of the IMAC purification can be performed in the presence of any suitable reducing agents. The reducing agent may be, but is not limited to, 2-mercaptoethanol, or TCEP (Tris[2-Carboxyethylphosphine] hydrochloride). Preferably, the reducing agent is about 2.0 mM TCEP.

[0188] The binding and contaminant removal steps of the IMAC purification may be performed in the presence of a detergent. The detergent may be, but is not limited to, CHAPS (3-([3-cholamidopropyl]-dimethylammonio)-1-propanesulfonate), Triton X-100, Nonidet P-40, Tween 20, or Tween 80. Preferably, the detergent is about 10.0 mM CHAPS.

[0189] The binding and contaminant removal steps of the IMAC purification may be performed in the presence of an ion source. The ion source may be, but is not limited to, KCl, NaCl, or sodium sulfate. Preferably, an ion source is about 0.3 M NaCl.

[0190] The elution of MEK2 from the IMAC resin may be accomplished by several modes, which are known in the art. For example, the elution of MEK2 from the IMAC column may be accomplished by using, for example, EDTA, histidine, or imidazole, or by reducing the pH. Preferably, the elution of MEK2 may be accomplished with about 0.1 M EDTA.

[0191] The elution step of the IMAC purification may be performed in the presence of any suitable buffering agent (s). The buffering agent may be, but is not limited to, Tris, phosphate, HEPES, or MOPS. Preferably, the buffering agent may be about 20.0 mM HEPES (pH of about 8.0). The elution of MEK2 also may be performed in the presence of any suitable organic agents. The organic agent may be, but is not limited to, glycerol or ethylene glycol. Preferably, the organic agent is about 10% glycerol.

[0192] The invention also provides a method for further purifying the protein using cation exchange chromatography, followed by concentration of the protein and size exclusion chromatography (SEC).

[0193] The cation exchange step may be performed using several types of chromatography resins. For example, the cation exchange resin may be, but is not limited to, S-Sepharose™, MonoS™, POROS™ HS, or POROS™ S. Preferably, the cation exchange resin is POROS™ HS. The cation exchange step may be performed in the presence of any suitable buffering agent(s). The buffering agent may include, but is not limited to, phosphate, malonic acid, butanedioic acid, acetic acid, MES (2-(N-morpholino)-ethanesulfonic acid), or HEPES. Preferably, the buffering agent is about 20.0 mM MES (pH of about 6.4).

[0194] The cation exchange step may be performed in the presence of any suitable reducing agent(s). The reducing agent may be, but is not limited to, 2-mercaptoethanol, TCEP, or dithiothreitol (DTT). Preferably, the reducing agent is about 2.0 mM TCEP.

[0195] The cation exchange step may be performed in the presence of any suitable organic agent(s). The organic agent may be, but is not limited to, glycerol or ethylene glycol. Preferably, the organic agent is about 20.0% ethylene glycol.

[0196] Elution of the MEK2 from the cation exchange resin may be accomplished by several different modes that are known in the art. For example, the MEK2 may be eluted by increasing the pH. Alternatively, the MEK2 may be eluted by increasing the salt concentration by using, for example, NaCl, KCl, ammonium acetate, or sodium sulfate. Preferably, ammonium acetate may be used to cause the elution by an increase the salt concentration.

[0197] The SEC step may be performed using various types of chromatography resins. For example, the suitable SEC resin may include, but is not limited to, Sephadex™ G-100, Sephadex™ G-200, Sephacryl™ S-100, Sephacryl™ S-200, Superdex™ 75, or Superdex™ 200. Preferably, the SEC resin is Superdex™ 200.

[0198] The SEC step may performed in the presence of any suitable buffering agent(s). The buffering agent may be, but is not limited to, phosphate, HEPES, MES, Tris, bis-Tris, or bis-Tris propane. Preferably, the buffering agent is about 20.0 mM HEPES (pH of about 7.5).

[0199] The SEC step may be performed in the presence of any suitable reducing agent(s). The reducing agent may be, but is not limited to, 2-mercaptoethanol, TCEP, or DTT. Preferably, the reducing agent is about 2.0 mM TCEP.

[0200] The SEC step may be performed in the presence of any suitable salt(s). The salt may be, but is not limited to, NaCl, KCl, ammonium acetate, or sodium sulfate. Preferably, the salt is about 150.0 mM ammonium acetate.

[0201] The SEC step may be performed in the presence of any suitable chelating agent(s). The chelating agent may be, but is not limited to, sodium citrate or EDTA. Preferably, the salt is about 0.1 mM EDTA.

[0202] The invention also provides a method for forming a MEK2: ligand complex. The MEK2: ligand complex formation may be performed at any point during the MEK2 purification. Preferably, the MEK2: ligand complex formation step may be performed following the SEC step. Alternatively, the MEK2: ligand complex formation step could be performed prior to the SEC step. The MEK2: ligand complex formation step may be performed using various concentrations of MEK2. For example, the concentration of MEK2 may be in the range of about 0.02 mg/ml to about 2 mg/ml. Preferably, the concentration of MEK2 is about 0.2 mg/ml to about 0.3 mg/ml. Further, the MEK2: ligand complex formation step may be performed at various molar ratios of MEK2 to ligand. For example, the molar ratio of MEK2 to ligand may be in the range of about 1:1 to about 1:1000. Preferably, the molar ratio of MEK2 to ligand is about 1:10.

Crystallization of Modified MEK1 and MEK2 Peptide Complexes

[0203] The present invention further includes methods of using modified MEK1 and MEK2 peptides, such as NH_2-terminally truncated MEK1 and MEK2 peptides, to grow crystals of a MEK1 or MEK2 peptide: ligand: cofactor complex. The crystallization conditions and methods listed herein are provided to elucidate one approach used in the crystallization of the MEK1 or MEK2 peptide: ligand: cofactor complexes. Of course those of ordinary skill in the art would be aware of other crystallization conditions and techniques that may be suitable for the crystallization of the modified MEK1 proteins described herein. For examples see, McPherson, A., Crystallization of Biological Macromolecules, Cold Spring Harbor Laboratory Press (1999).

Crystallization of Modified MEK1 Peptide Complexes

[0204] Generally, the crystallization of modified MEK1 peptide complexes comprises contacting a NH_2-terminally truncated MEK1 peptide with a ligand and a cofactor, wherein a stable ternary complex of a MEK1 peptide: ligand: cofactor is formed, and then growing a crystal of the MEK1 peptide: ligand: cofactor complex by adding the solution of the ternary complex to a precipitating solution. For example, in order to produce crystals of a MEK1 peptide: ligand: cofactor complex, a solution ("MEK1 solution") containing the MEK1 peptide, a ligand and a cofactor and a precipitant solution are provided. The concentration of MEK1 in the MEK1 solution is from about 2 mg/mL to about 40 mg/mL, preferably from about 10 mg/mL to about 20 mg/mL, and more preferably is about 15 mg/mL. The concentration of ligand is from about 2- and about 20-fold in excess that of the MEK1 concentration, preferably, is from about 5- and about 15-fold in excess that of the MEK1 concentration, and more preferably, is about 10-fold excess. The concentration of cofactor in the MEK1 solution is from about 1 mM to about 100 mM, preferably from about 2.5 mM to about 25 mM and, more preferably, is about 5 mM.

[0205] The cofactor may include, but is not limited to, an ATP-cation, non-hydrolyzable ATP analogue such as AMP-PNP (adenylyl-imidodiphosphate), or ATP-Gamma-S (Adenosine 5'-O-3-thiotriphosphate). The ATP-cation may include, but is not limited to, a lithium, sodium, magnesium, or potassium salt of ATP. Preferably, the ATP-cation is a sodium or magnesium salt of ATP. More preferably, the ATP-cation is a magnesium salt of ATP ("Mg-ATP").

[0206] The MEK1 solution may comprise, but is not limited to, MEK1, ligand, cofactor, a buffering agent, a reducing agent and a source of ionic strength. The concentrations of the protein, ligand and cofactor are described above. The buffering agent may be, but is not limited to, phosphate, MES, HEPES (N-2-hydroxyethyl-piperazine-N'-2-ethanesulfonic acid), Tris, bis-Tris, or bis-Tris propane. Preferably, the buffering agent is HEPES of a concentration between about 10 mM and about 100 mM and a pH value between about 6.8 and about 8.8. More preferably, the buffering agent is about 20 mM HEPES (pH 7.8). The reducing agent may be, but is not limited to, 2-mercaptoethanol, TCEP or DTT. Preferably, the reducing agent is TCEP at a concentration between about 0.1 mM and about 10 mM. More preferably, the reducing agent is about 2.0 mM TCEP. The MEK1 solution may contain a salt as source of ionic strength. The salt may be, but is not limited to, NaCl KCl, ammonium acetate or sodium sulfate. Preferably, the salt is ammonium acetate at a concentration between about 5 mM and about 500 mM. More preferably, the salt is about 150 mM ammonium acetate.

[0207] The MEK1 solution may optionally contain any suitable chelating agent(s). The chelating agent may be sodium citrate. When the MEK1 solution contains a chelating agent, about 0.5 mM EDTA is preferably used as the chelating

agent.

[0208] In addition, any precipitating solution ("MEK1 precipitant solution") may also be used in the crystallization of MEK1 peptide : ligand : cofactor complex. When mixed with the MEK1 solution described above, the precipitating solution preferably causes the ternary complex to form well-diffracting crystals. The MEK1 precipitant solution may comprise a variety of components designed to stabilize the formation of the MEK1 peptide: ligand: cofactor complex as a crystalline solid. For example, the precipitant solution may include, but is not limited to, a source of ionic strength, a source of polyethylene glycol (PEG), a buffering agent, and a reducing agent.

[0209] The buffering agent of the MEK1 precipitant solution may be, but is not limited to, phosphate, acetate, succinate, malonate, malate, imidazole, MES, Tris, or bis-Tris propane, or any combination thereof. Preferably, the buffering agent is a mixed buffer system of imidazole/ malate/ phosphate buffer. The concentrations of the buffers may be in the ranges of about 1 mM - about 100 mM for imidazole, about 10 mM - about 1000 mM for malate, and about 40 mM - about 1400 mM for phosphate. The mixed buffer system may have a pH value between about pH 3.0 and about pH 7.0. For the phosphate buffer, ammonium phosphate monobasic may be preferably used. Most preferably, the mixed buffer system comprises about 10 mM imidazole, about 100 mM malate, and about 400 mM ammonium phosphate and has a pH value between about pH 4.5 and about pH 5.5.

[0210] The source of ionic strength of the MEK1 precipitant solution may be, but is not limited to, NaCl, KCl, ammonium sulfate, lithium sulfate, ammonium phosphate, or sodium potassium phosphate. The mixed buffer system of the MEK1 precipitant solution may serve as an ionic strength source. Preferably, monobasic ammonium phosphate is added, without adjustment of the pH, to a concentration of 100 -1000 mM, or more preferably to a concentration of 200 - 600 mM to a solution of the 10 mM imidazole/100 mM malate acid buffer solution that has had the pH value adjusted to pH 7.0 with a 50% (v/v) solution of KOH. The resulting solution preferably has the appropriate ionic strength and a final pH value in the range of about pH 4.5 to about pH 5.5.

[0211] The MEK1 precipitant solution also may contain any suitable reducing agent(s). The reducing agent may include, but is not limited to, 2-mercaptoethanol, TCEP or DTT at a concentration of about 0.1 mM to about 100 mM. Preferably, DTT may be used. Most preferably, about 20 mM DTT may be used.

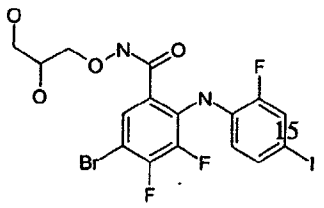
[0212] Many possible method could be used to grow the crystals of the MEK1 peptide: ligand: cofactor complex, including, but is not limited to, hanging-drop vapor diffusion, sitting-drop vapor diffusion, microbatch, batch, or counter diffusion in gels or oils. Preferably, the crystallization may be performed by hanging-drop vapor diffusion. When using the method of hanging drop vapor diffusion to grow the MEK1: ligand: cofactor crystals, the MEK1 solution is mixed with a droplet of the MEK1 precipitant solution to obtain a mixed droplet solution. The mixed droplet solution is then suspended over a well of precipitant solution in a sealed container. For example, about 1 μL of the MEK1 solution is mixed with the MEK1 precipitant solution in a ratio from about 1:4 to about 4:1, and preferably from about 1:2 to about 2:1. More preferably, the ratio of the MEK1 solution to the MEK1 precipitant solution is about 1:1. In one embodiment, the mixed droplet may be suspended over a well solution containing between 0.6 mL and 1.2 mL, and more preferably about 1.0 mL of precipitant solution. The crystallization temperature may be between about 4°C and about 20°C, preferably is about 13°C, and more preferably the crystals are grown at 13°C for 3-5 days and then moved to room temperature.

[0213] The mixed droplet solution is allowed to stand suspended over the well solution containing the MEK1 precipitant solution at the temperature described above for a period of about 5 days to about 5 weeks until the MEK1 peptide: ligand: cofactor crystals reach a size appropriate for crystallographic data collection, preferably between about 0.05 x about 0.05 x about 0.1 mm to about 0.3 x about 0.3 x about 0.5 mm.

[0214] Standard micro and/or macro seeding may also be used to obtain a crystal of X-ray diffraction quality, i.e. a crystal that will diffract to a resolution greater than 5.0 Å. In the preferred form, no seeding is used to grow diffraction quality crystals.

[0215] After the desired growth is achieved, the crystals of MEK1 peptide: ligand: cofactor complex, may be harvested and bathed in a cryoprotective solution. The cryoprotective solution may comprise a variety of components designed to stabilize the formation of a vitreous solid containing the MEK1 peptide: ligand: cofactor complex as a crystalline solid at a temperature of about 110 Kelvin. The cryoprotective solution may comprise, but is not limited to, a suitable source of low molecular weight solution of ethylene glycol or polyethylene glycol (PEG), a diluting agent and a cryo oil solution made up of about 70% Paratone-N oil and 30% mineral oil. The low molecular weight ethylene glycol or polyethylene glycol solution may have a molecular weight of about 100 to about 1000, more preferably about 200 to 600, and most preferably a 100% solution of ethylene glycol is used. The ethylene glycol or PEG may be used as a 100% (w/v) solution and then diluted with the crystallization well solution to a final concentration of between 5 and 25%. Most preferably the PEG solution will be made to a final concentration of 10% with the well solution. During the cryo preparation process, the crystal may first be removed from the mother liquor and then bathed in the 10% PEG solution for 1 -20 minutes. Most preferably the crystal will placed in the PEG/ well solution for about 2 minutes. The crystal may then be removed to a Paratone-N and mineral oil mixture and manipulated to in the oil to remove the aqueous solution prior to quickly placing the cryo-protected crystal into a liquid nitrogen bath.

[0216] Although any ligand for the NH_2-terminally truncated MEK1 peptide may be used, preferably the ligand comprises a MEK1 or MEK2 inhibitor. Preferably, the ligand is 5-bromo-N-(2,3-dihydroxy-propoxy)-3,4-difluoro-2-(2-fluoro-4-iodo-phenylamino)-benzamide having the following chemical structure:



[0217] A crystal of the present invention may take a variety of crystal forms, all of which are included in the present invention. In one embodiment the crystals may be triclinic, monoclinic, orthorhombic, tetragonal, cubic, trigonal or hexagonal. In a preferred embodiment the crystal has hexagonal symmetry. In a more preferred embodiment the crystal has hexagonal symmetry and has the space group $P6_2$. In the most preferred form the crystal has the space group $P6_2$ and has a unit cell consisting of approximately: $a = b = 81.4 \pm 0.3$ Å; $c = 129.0 \pm 0.3$ Å; $\alpha = \beta = 90.0°$; $\gamma = 120.0°$.

Crystallization of Modified MEK2 Peptide Complexes

[0218] Generally, the crystallization of modified MEK2 peptide complexes comprises contacting a NH_2-terminally truncated MEK2 peptide with a ligand and a cofactor, wherein a stable ternary complex of a MEK2 peptide: ligand: cofactor is formed, and then growing a crystal of the MEK2 peptide: ligand: cofactor complex by adding the solution of the ternary complex to a precipitating solution. For example, in order to produce crystals of a MEK2 peptide: ligand: cofactor complex, a solution ("MEK2 solution") containing the MEK2 peptide, a ligand and a cofactor and a precipitant solution are provided. The concentration of MEK2 in the MEK2 solution is from about 2 mg/mL to about 40 mg/mL, preferably from about 10 mg/mL to about 20 mg/mL, and more preferably is about 15 mg/mL. The concentration of ligand is from about 2- and about 20-fold in excess that of the MEK2 concentration, preferably, is from about 5- and about 15-fold in excess that of the MEK2 concentration, and more preferably, is about 10-fold excess. The concentration of cofactor in the MEK2 solution is from about 1 mM to about 100 mM, preferably from about 2.5 mM to about 25 mM and, more preferably, is about 5 mM.

[0219] The cofactor may include, but is not limited to, an ATP-cation, non-hydrolyzable ATP analogue such as AMP-PNP (adenylyl-imidodiphosphate), or ATP-Gamma-S (Adenosine 5'-O-3-thiotriphosphate). The ATP-cation may include, but is not limited to, a lithium, sodium, magnesium, or potassium salt of ATP. Preferably, the ATP-cation is a sodium or magnesium salt of ATP. More preferably, the ATP-cation is a magnesium salt of ATP ("Mg-ATP").

[0220] The MEK2 solution may comprise, but is not limited to, MEK2, ligand, cofactor, a buffering agent, a reducing agent and a source of ionic strength. The concentrations of the protein, ligand and cofactor are described above. The buffering agent may be, but is not limited to, phosphate, MES, HEPES (N-2-hydroxyethyl-piperazine-N'-2-ethanesulfonic acid), Tris, bis-Tris, or bis-Tris propane. Preferably, the buffering agent is HEPES of a concentration between about 10 mM and about 100 mM and a pH value between about pH 6.8 and about pH 8.8. More preferably, the buffering agent is about 20 mM HEPES (pH 7.5). The reducing agent may be, but is not limited to, 2-mercaptoethanol, TCEP or DTT. Preferably, the reducing agent is TCEP at a concentration between about 0.1 mM and about 10 mM. More preferably, the reducing agent is about 2.0 mM TCEP. The MEK2 solution may contain a salt as source of ionic strength. The salt may be, but is not limited to, NaCl, KCl, ammonium acetate or sodium sulfate. Preferably, the salt is ammonium acetate at a concentration between about 5 mM and about 500 mM. More preferably, the salt is about 150 mM ammonium acetate.

[0221] The MEK2 solution may optionally contain any suitable chelating agent(s). The chelating agent may be sodium citrate. When the MEK2 solution contains a chelating agent, about 0.1 mM EDTA is preferably used as the chelating agent.

[0222] In addition, any precipitating solution ("MEK2 precipitant solution") may also be used in the crystallization of MEK2 peptide : ligand : cofactor complex. When mixed with the MEK2 solution described above, the precipitating solution preferably causes the ternary complex to form well-diffracting crystals. The MEK2 precipitant solution may comprise a variety of components designed to stabilize the formation of the MEK2 peptide: ligand: cofactor complex as a crystalline solid. For example, the precipitant solution may include, but is not limited to, a source of ionic strength, a buffering agent, and a reducing agent.

[0223] The buffering agent of the MEK2 precipitant solution may be, but is not limited to, sodium / potassium phos-

phate, ammonium phosphate, acetate, imidazole, MES, HEPES, Tris, or bis-Tris propane, or any combination thereof. Preferably, the buffering agent is also the source of ionic strength using a mixed solution of sodium monobasic phosphate and potassium dibasic phosphate buffered to about pH 6 to about pH 8. The concentration of the sodium potassium phosphate buffer may preferably be in the range of about 1.4 to about 1.9 M sodium monobasic phosphate and potassium dibasic phosphate. Most preferably, the mixed phosphate buffer system may be in the range of about 1.4 to about 1.9 M sodium monobasic phosphate and potassium dibasic phosphateand buffered to about pH 6.7 to about pH 7.1.

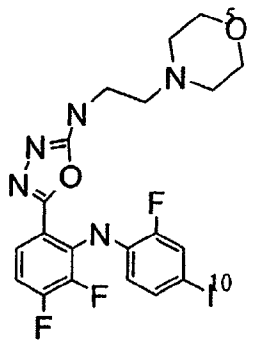
[0224] The MEK2 precipitant solution also may contain any suitable reducing agent(s). The reducing agent may include, but is not limited to, 2-mercaptoethanol, TCEP or DTT at a concentration of about 0.1 mM to about 100 mM. Preferably, DTT may be used. Most preferably, about 20 mM DTT may be used.

[0225] Many possible method could be used to grow the crystals of the MEK2 peptide: ligand: cofactor complex, including, but is not limited to, hanging-drop vapor diffusion, sitting-drop vapor diffusion, microbatch, batch, or counter diffusion in gels or oils. Preferably, the crystallization may be performed by hanging-drop vapor diffusion. When using the method of hanging drop vapor diffusion to grow the MEK2: ligand: cofactor crystals, the MEK2 solution is mixed with a droplet of the MEK2 precipitant solution to obtain a mixed droplet solution. The mixed droplet solution is then suspended over a well of precipitant solution in a sealed container. For example, about 1 μL of the MEK2 solution is mixed with the MEK2 precipitant solution in a ratio from about 1:4 to about 4:1, and preferably from about 1:2 to about 2:1. More preferably, the ratio of the MEK2 solution to the MEK2 precipitant solution is about 1:1. In one embodiment, the mixed droplet may be suspended over a well solution containing between 0.6 mL and 1.2 mL, and more preferably about 1.0 mL of precipitant solution. The crystallization temperature may be between about 4°C and about 20°C, and preferably is about 13°C. The mixed droplet solution is allowed to stand suspended over the well solution containing the MEK2 precipitant solution at the temperature described above for a period of about 5 days to about 5 weeks until the MEK2 peptide: ligand: cofactor crystals reach a size appropriate for crystallographic data collection, preferably between about 0.05 x about 0.05 x about 0.1 mm to about 0.3 x about 0.3 x about 0.5 mm.

[0226] Standard micro and/or macro seeding may also be used to obtain a crystal of X-ray diffraction quality, i.e. a crystal that will diffract to a resolution greater than 5.0 Å. In the preferred form, no seeding is used to grow diffraction quality crystals.

[0227] After the desired growth is achieved, the crystals of MEK2 peptide: ligand: cofactor complex, may be harvested and bathed in a cryoprotective solution. The cryoprotective solution may comprise a variety of components designed to stabilize the formation of a vitreous solid containing the MEK2 peptide: ligand: cofactor complex as a crystalline solid at a temperature of about 110 Kelvin. The cryoprotective solution may comprise, but is not limited to, a low molecular weight polyethylene glycol (PEG), glycerol or ethylene glycol, and / or a cryo oil solution made up of about 70% Paratone-N oil and 30% mineral oil. The cryo solution may be used by combining the ethylene glycol with the Paratone-N and mineral oil mixture as was done with MEK1 or by using either the Paratone-N / mineral oil mixture or the ethylene glycol independently. In a preferred form, the ethylene glycol was used at a concentration of about 5 -30% made by mixing a 100% solution of ethylene glycol with the well solution from the crystallization condition. In the most preferred form, the crystals may be removed from the mother-liquor crystal growth solution directly to the Paratone-N and mineral oil mixture using a mounted loop and manipulated in the oil to remove the aqueous solution prior to quickly placing the cryo-protected crystal into a liquid nitrogen bath.

[0228] Although any ligand for the NH_2-terminally truncated MEK2 peptide may be used, preferably the ligand comprises a MEK2 or MEK2 inhibitor. Preferably, the ligand is {5-[3,4-Difluoro-2-(2-fluoro-4-iodo-phenylamino)-phenyl]-1,3,4-oxadiazol-2-yl}-(2-morpholin-4-yl-ethyl)-amine having the following chemical structure:



[0229] A crystal of the present invention may take a variety of crystal forms, all of which are included in the present invention. In one embodiment the crystals may be triclinic, monoclinic, orthorhombic, tetragonal, cubic, trigonal or hexagonal. In a preferred embodiment the crystal has hexagonal symmetry. In a more preferred embodiment the crystal has hexagonal symmetry and has the space group $P6_122$. In the most preferred form the crystal has the space group $P6_122$ and has a unit cell consisting of approximately: $a = b = 161.89 \pm 0.3$ Å; $c = 122.99 \pm 0.3$ Å; $\alpha = \beta = 90.0°$; $\gamma = 120.0°$.

X-ray data collection and structural determination

[0230] The present invention further includes methods for collecting X-ray diffraction data on the MEK1 and MEK2 peptide: ligand: cofactor crystals. The data collection conditions and methods listed herein are provided to elucidate the approach used for structural determination of the MEK1 and MEK2 peptide: ligand: cofactor crystals. Of course those of ordinary skill in the art would be aware of other conditions and techniques that may be suitable for the X-ray data collection and structural determination of the modified MEK1 or MEK2 protein crystals described herein. For examples see, Glusker, J., Crystal Structure Analysis for Chemists and Biologists, Wiley-VCH Press (1994) or the International Tables for X-Ray Crystallography, Volume F, edited by M.G. Rosssman and E. Arnold, Kluwer Academic Publishers (2001).

[0231] Generally, collecting the X-ray diffraction data for the MEK1 or MEK2 peptide: ligand: cofactor complex crystals comprises mounting the crystals in a cryo loop, bathing the crystals in a cryo protectant solution, rapidly cooling the crystals to about 100 K and collecting diffraction data in the oscillation mode. The source of X-rays may be, but is not limited to, a rotating anode home source such as a Rikagu RU-H3R generator, or a high energy synchrotron source such as that found on beamline 17 (17-ID or 17-BM, IMCA-CAT) at the Argonne National Laboratory Advanced Photon Source. The preferred method of data collection is to collect an initial data set using the home source to evaluate the crystal quality and then collecting a complete data set at IMCA-CAT. The method of detecting and quantitating the diffraction data may be performed by using, for example, an image plate such as a R-Axis IV^{++} from MSC/Rigaku, or a charge-coupled device like a MAR-CCD, or ADSC Quantum 210 X-ray detector. Preferably, the resulting MEK1 crystal diffracts X-rays for the determination of the atomic coordinates of the MEK1 peptide: ligand: cofactor complex, to a resolution better than 5.0 Å, more preferably to a resolution better than 3.0 Å, and even more preferably to a resolution of better than 2.5 Å. Preferably, the resulting MEK2 crystal diffracts X-rays for the determination of the atomic coordinates of the MEK2 peptide: ligand: cofactor complex, to a resolution better than 5.0 Å, more preferably to a resolution better than 3.5 Å.

[0232] Once the data is collected, it is generally corrected for Lorenz and polarization effects and converted to indexed structure factor amplitudes using data processing software, for example DENZO or HKL2000 (Otwinowski, Z. and Minor, W., Processing of X-ray diffraction data collected in oscillation mode, *Methods Enzymol.* 276: 307-326 (1997)), d*Trek (Rigaku MSC) or Mosfilm (Leslie, A.G.W., Joint CCP4 + ESF-EAMCB Newsletter on Protein Crystallography, No. 26 (1992)). The preferred processing software may be HKL2000. The scaled and reduced diffraction data from the crystal may be used to determinae the three-dimensional crystal structure using one or more of the following methods or by other similar methods not included in this list: Fourier difference methods, molecular replacement (MR), multiwavelength anomalous dispersion (MAD), single-wavelength anomalous dispersion (SAD), single isomorphous replacement with anomalous scattering (SIRAS) or multiple isomorphous replacement (MIR).

MEK1 and MEK2 Crystallographic Structural Analysis

[0233] The present invention further includes methods for solving the three-dimensional structural coordinates of the MEK1 and MEK2 peptide: ligand: cofactor crystalline complexes using the X-ray diffraction data. The methods used for structural determination are provided to elucidate the approach used for the structural determination of the crystalline MEK1 and MEK2 peptide: ligand: cofactor crystalline complexes. Those of ordinary skill in the art would be aware of other conditions and techniques that may be suitable for the X-ray structural determination of the modified MEK1 and MEK2 protein complexes described herein. For examples see, Glusker, J., Crystal Structure Analysis for Chemists and Biologists, Wiley-VCH Press (1994) or the International Tables for X-Ray Crystallography, Volume F, edited by M. G. Rosssman and E. Arnold, Kluwer Academic Publishers (2001)..

[0234] In the structural determination of the first MAPK kinase, it was necessary to use methods other than molecular replacement to solve the phase problem. In this case, an iodine atom contained within the bound ligand/inhibitor was used for SAD phase estimation. Other methods like MIR, MAD or SAD could have alternatively been used. In a preferred embodiment, the data may be scaled isomorphously using the SCALEPACK module in HKL2000 (Otwinowski et al, *Methods Enzymol.* 276:307-326 (1997)). Alternatively, the data could have been scaled using d*Trek (Rigaku MSC), or SCALA (COLLABORATIVE COMPUTATIONAL PROJECT, No. 4, "The CCP4 Suite: Programs for Protein Crystallography" *Acta Cryst.* D50, 760-763 (1994)). All subsequent calculations may be done using the CNX package (Accelrys, San Diego, CA.). Alternatively, the structural coordinates could have been identified using the CCP4 program

suite, or a combination of other software packages known to those skilled in the art.

[0235] After the structures of MEK1 and MEK2 were solved, the three-dimensional structures were prepared for use in structure-based drug design. The preparation and analysis of the MEK1 and MEK2 templates may be performed by using, for example, SYBYL®, GRIN/GRID®, MolCad®, GOLD®, FlexX®. Additionally, suitable computer modeling software can optionally be used to perform structural determination. Such software includes, but is not limited to, QUANTA® (Accelrys, San Diego, CA), CHARMm® (Accelrys), INSIGHT® (Accelrys), SYBYL® (Tripos, Inc., St. Louis), MacroModel® (Schrödinger, Inc.) and ICM (MolSoft, LLC), with SYBYL® being the most preferable program. The computer program may be used alone or combined with a docking computer program such as GRAMM (Ilya A. Vakser, Rockefeller Univ.), FlexX® (Tripos Inc.), Flexidock® (Tripos Inc.), GOLD (commercially available via Cambridge Crystallographic Data Centre, Cambridge, UK), DOCK (Irwin Kuntz, Department of Pharmaceutical Chemistry at the University of California, San Francisco), or AutoDock® (Molecular Graphics Laboratory). These docking computer programs scan known databases of small molecules to find core compounds that roughly fit the binding sites. GOLD® may most preferably be used

[0236] If necessary, crystallographic data in PDB (Protein DataBank) files can be "cleaned up" by modifying the atom types of the inhibitor and cofactor and any water molecules that are present so that the water molecules find their lowest energy rotamer. Suitable software for performing this "clean up" include, but are not limited to, SYBYL®, WATCHECK (part of CCP4 suite, COLLABORATIVE COMPUTATIONAL PROJECT, No. 4, "The CCP4 Suite: Programs for Protein Crystallography." *Acta Cryst.* D50, 760-763 (1994)), and REDUCE (Word, *et al.*, "Asparagine and glutamine: using hydrogen atom contacts in the choice of side chain amide orientation" *J. Mol. Bio.* 285: 1733-45 (1999)), with REDUCE, or any software performing the equivalent function as REDUCE, being the most preferred software. Any suitable docking computer program may be used to further validate the refined protein structure by adding all of the hydrogens in the most favorable protonation state as well as rotating all water molecules into orientations that give the optimal interactions with the protein.

[0237] Further, the binding sites may be characterized using, for example, GRIN/GRID® (Molecular Discovery Limited), MOLCAD® (Tripos, Inc.) contouring, CAVEAT (P.A. Bartlett, *et al.*, CAVEAT: A program to facilitate the structure-derived design of biologically active molecules, in molecular recognition in chemical and biological problems, special Publication, *Royal Chem. Soc.*, 78, 182-196 (1989), available from the University of California, Berkely, CA), GRASP (A. Nicholls, Columbia Unviersity), SiteID® (Tripos, Inc.), INSIGHT®, or SYBYL®. These softwares may be used individually or in combination. For example, the combination of GRID/GRID®, MolCad® (Tripos, Inc.) and SYBYL® may be preferably used.

[0238] According to one embodiment of the invention, it has been discovered that the MEK1 peptide comprises a ligand-binding pocket that is defined by the structural coordinates of the following amino acid residues within 4 Å of a MEK1 inhibitor located in the ligand-binding site: G77, N78, G79, G80, K97, I99, L115, L118, V127, F129, I141, M143, C207, D208, F209, G210, V211, S212, L215, I216, M219 of SEQ ID NO: 2; or by structural coordinates of the following amino acid residues within 5 Å of a MEK1 inhibitor located in the ligand-binding site: G77, N78, G79, G80, K97, I99, L115, L118, I126, V127, G128, F129, I141, M143, D190, N195, L206, C207, D208, F209, G210, V211, S212, L215, I216, M219, F223 of SEQ ID NO: 2.

[0239] Further, it has been discovered that the MEK1 peptide comprises a cofactor-binding pocket that is defined by the structural coordinates of the following residues within 4 Å of the ATP molecule in the cofactor-binding site: L74, G75, A76, G77, N78, G80, V81, V82, A95, K97, V127, M143, E144, H145, M146, G149, S150, D152, Q153, K192, S194, N195, L197, D208, V224 of SEQ ID NO: 2; or structural coordinates of the following residues within 5 Å of the ATP molecule in the cofactor-binding site: L74, G75, A76, G77, N78, G79, 80, V81, V82, A95, K97, V127, M143, E144, H145, M146, D147, G149, S150, D152, Q153, D190, K192, S194, N195, L197, C207, D208, V224, G225 of SEQ ID NO: 2.

[0240] It has also been discovered that the MEK2 peptide comprises a ligand-binding pocket that is defined by the structural coordinates of the following amino acid residues within 4 Å of a MEK2 inhibitor located in the ligand-binding site: G81, N82, G83, G84, K101, I103, L119, L122, V131, F133, I145, M147, C211, D212, F213, G214, V215, S216, L219, I220, M223 of SEQ ID NO: 4, or a conservatively substituted variant thereof; and is defined by structural coordinates of the following amino acid residues within 5 Å of a MEK2 inhibitor located in the ligand-binding site: G81, N82, G83, G84, K101, I103, L119, L122, I130, V131, G132, F133, I145, M147, D194, N199, L210, C211, D212, F213, G214, V215, S216, L219, I220, M223, F227 of SEQ ID NO: 4, or a conservatively substituted variant thereof.

[0241] Additionally, it has been discovered that the MEK2 peptide comprises a co-factor-binding pocket that is defined by the structural coordinates of the following residues within 4 Å of the ATP molecule in the cofactor-binding site: L78, G79, A80, G81, N82, G84, V85, V86, A99, K101, V131, M147, E148, H149, M150, G153, S154, D156, Q157, K196, S198, N199, L201, D212, V228 of SEQ ID NO: 4, or a conservatively substituted variant thereof; and is defined by the structural coordinates of the following residues within 5 Å of the ATP molecule in the cofactor-binding site: L78, G79, A80, G81, N82, G83, G84, V85, V86, A99, K101, V131, M147, E148, H149, M150, D151, G153, S154, D156, Q157, D194, K196, S198, N199, L201, C211, D212, V228, G229 of SEQ ID NO: 4, or a conservatively substituted variant

thereof.

[0242] Those of skill in the art will recognize that a set of structural coordinates for a peptide or a peptide: ligand: cofactor complex or a subset thereof, is a relative set of points in space that defines a complex three dimensional surface. As such it is possible to represent the same surface using an entirely different set of coordinates. Also, due to small errors in the measurement of all crystallographic data, slight variations in the individual coordinates will have little or no effect on the overall surface. Thus, a binding pocket could be generated from the structural coordinates provided in Table 1 or Table 2 from some variation of the structural coordinate that still retains similar surface features, including, but not limited to, volume (both internally in cavities or in total), solvent accessibility, and surface charge and hydrophobicity. In addition, the structural coordinates could be modified by crystallographic permutations, including, but not limited to, fractionalization, integer addition or substraction, inversion or any combination thereof.

[0243] In addition, it would be apparent to one skilled in the art that the binding pockets described in detail above could be modified in order to obtain somewhat different three-dimesional coordiates.

[0244] It should also be recognized that minor modification of any or all of the components of the peptide: ligand: cofactor complexes that results in the generation of structural coordinates that still retains the basic features of the three-dimensional structure should be considered part of the invention.

Computers, Computer Software, Computer Modeling

[0245] Once the atomic coordinates are known, a computer may be used for producing a three-dimensional representation of a MEK1 peptide, a MEK2 peptide, or a structurally related peptide. Likewise, the atomic coordinates, or related set of structural coordinates, may be used to generate a three dimensional represenation of a MEK1 peptide binding pocket, MEK-2 peptide binding pocket or MEK-like peptide binding pocket. Thus, another aspect of the invention involves using the structural coordinates generated from the MEK1 and MEK2 complexes as set forth in Table 1 or Table 2, or a related set of structural coordinates, to generate three-dimensional representations of MEK1 peptide, MEK2 peptide, or a structurally related peptide, or a MEK1, MEK2, or MEK-like peptide binding pocket. This is achieved through the use of commercially available software that is capable of generating three-dimensional graphical representations of molecules or portions thereof from a set of atomic coordinates.

[0246] Suitable computers are known in the art and typically include a central processing unit (CPU), and a working memory, which can be random-access memory, core memory, mass-storage memory, or a combination thereof. The CPU may encode one or more programs. Computers also typically include display, input and output devices, such as one or more cathode-ray tube display terminals, keyboards, modems, input lines and output lines. Further, computers may be networked to computer servers (the machine on which large calculations can be run in batch) and file servers (the main machine for all the centralized databases).

[0247] Machine-readable media containing data, such as the atomic coordinates set forth in Table 1 and Table 2, or a related set of atomic coordinates, may be inputted using various hardware, including modems, CD-ROM drives, disk drives, or keyboards.

[0248] Machine-readable data medium can be, for example, a floppy diskette, hard disk, or an optically-readable data storage medium, which can be either read only memory, or rewritable, such as a magneto-optical disk.

[0249] Output hardware, such as a CRT display terminal, may be used for displaying a graphical representation of the three-dimensional structural coordinates of the MEK1 or MEK2 peptides as set forth in Tablel or Table 2 respectively, of a structurally related peptide, or of a MEK1, MEK2, or MEK-like binding pocket, as described herein. Output hardware may also include a printer and disk drives.

[0250] The CPU coordinates the use of the various input and output devices, coordinates data access from storage and access to and from working memory, and determines the sequence of data processing steps. A number of programs may be used to process the machine-readable data. Such programs are discussed herein in reference to the computational methods of drug discovery.

[0251] In a preferred embodiment of the invention, atomic coordinates capable of being processed into a three-dimensional representation of a molecule or molecular complex that comprises a MEK1, MEK2, or MEK-like peptide binding pocket are stored in a machine-readable storage medium. As described below, the three-dimensional structure of a molecule or molecular complex comprising a MEK1, MEK2, or MEK-like peptide binding pocket is useful for a variety of purposes, such as in drug discovery and drug design. For example, the three-dimensional structure derived from the atomic coordinate data may be computationally evaluated for its ability to associate with chemical entities.

MEK1 or MEK2 Activity Inhibitors and/or Enhancers

[0252] The association of natural ligands with their corresponding binding pockets on receptors or enzymes is the basis of many biological mechanisms of action. Similarly, many drugs exert their biological effects *via* an interaction with the binding pockets of a receptor or enzyme. An understanding of such associations can lead to the design of

drugs having more favorable and specific interactions with their target receptors or enzymes, and thus, improved biological effects. Therefore, information related to ligand association with the MEK1, MEK2, or MEK-like peptide binding sites is valuable in designing and/or identifying potential inhibitors or enhancers of MEK1, MEK2, or peptides structurally related thereto. Further, the more specific the design of a potential drug, the more likely that the drug will not interact with similar proteins, thus, minimizing potential side effects due to unwanted cross interactions.

[0253] Computer programs can be employed to estimate the attraction, repulsion, and steric hindrance of a ligand to a MEK1, MEK2, or MEK-like binding pocket. For example, one can screen computationally small molecule databases for chemical entities or compounds that can bind in whole, or in part, to a MEK1, MEK2, or MEK-like binding pocket. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity or by estimated interaction energy (Meng, et al., *J. Comp. Chem., 13*:505-524 (1992)). Generally, the tighter the fit, e.g., the lower the steric hindrance and/or the greater the attractive force, the more potent the drug is projected to be since these properties are consistent with a tighter-binding constant.

[0254] The present invention provides methods for screening candidate compounds as potential therapeutic agents for the treatment of various diseases associated with MEK1 and MEK2, including, but not limited to, disease states that involve diverse cellular processes including, but not limited to, apoptosis, differentiation, angiogenisis and inflammation. Such disease states include, for example, cancer, psoriasis, arthritis, septic shock, viral infections and cardiovascular disease.

[0255] More specifically, the present invention provides methods of using the three-dimensional representations of the MEK1, MEK2, and structurally related peptides, or binding pockets thereof, generated from the X-ray crystallographic data, or a related set of structural coordinates, to model the binding of candidate compounds. The methods include methods for screening and identifying potential inhibitors or enhancers of MEK1, MEK2, or a structurally peptide; and for the design of or modification of chemical entities having the potential to associate with MEK1, MEK2, a structurally related peptide, or binding pocket thereof.

[0256] The compound design or modification process begins after the structure of the target, e.g., a MEK1 or MEK2 peptide, is resolved to of greater than 5.0 Å, preferably greater than 3.5 Å. As described above, the data generated from the resolved crystal structure is applied to a computer algorithm to generate a three-dimensional representation and, ultimately, model, of the MEK1, MEK2 or structurally related peptide and MEK1, MEK2, MEK-like peptide binding pockets. Resolving the MEK1 and MEK2 three-dimensional structures using the X-ray crystallographic coordinates, as described above, enables one to determine whether a compound could occupy the ligand or cofactor binding site, as demonstrated in Figures 4 and 5, or a MEK-like binding pocket.

[0257] After a three-dimensional representation of the MEK1 or MEK2 petpide molecule, a structurally related peptide molecule, or a MEK1, MEK2 or MEK-like binding pocket is generated, a ligand having the potential to associate with the peptide or binding pocket is generated by, for example, (i) assembling molecular fragments into the chemical entity; (ii) de novo design of the chemical entity; (iii) selecting a chemical entity from a small molecule database; or (iv) modifying a known inhibitor, or portion thereof, of MEK1 or MEK2 activity.

[0258] If a chemical entity is designed, the following factors may be considered. First, the entity must be capable of physically and structurally associating with some or the entire MEK1, MEK2, or MEK-like binding pocket. Second, the entity must be able to assume a conformation that allows it to associate with a MEK1, MEK2, or MEK-like binding pocket directly. Although certain portions of the entity will not directly participate in these associations, those portions of the entity may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity in relation to all or a portion of the binding pocket, and the spacing between functional groups of an entity comprising several chemical entities that directly interact with the MEK1, MEK2, or MEK-like binding pocket.

[0259] The design of new compounds or the modification of known compounds may involve synthesizing or modifying compounds, or fragments thereof, *via* computer programs which build and link fragments or atoms into a target binding site(s) based upon steric and electrostatic complementarity, without reference to substrate analog structures. The computer program analyzes molecular structure and interactions. The computer analysis can be performed, for example, with one or more of the following computer programs: QUANTA®, CHARMM®, INSIGHT®, SYBYL®, MACROMODEL® or ICM [Dunbrack *et al.*, 1997, supra]. Selected compounds, or fragments thereof, may be positioned in a variety of orientations, or docked, within the MEK1, MEK2, or MEK-like binding pocket(s) as defined by the atomic coordinates. If compounds have been selected, then they may be assembled into a single complex. If fragments have been selected, then they may be assembled into a single compound. Assembly may be preceded by visual inspection of the relationship of the compounds or fragments to each other on the three-dimensional MEK1, MEK2, or MEK-like peptide binding pocket representation displayed on a computer screen in relation to the atomic coordinates. This visual image step may be followed by manual model building using appropriate software programs. Alternatively, compounds may be designed as a whole using either empty binding pocket(s) or binding pocket(s) containing the natural ligand(s).

[0260] Computer programs that may be used in the design or modification of the potential ligand include, but are not limited to, alone or in combination, QUANTA (Accelrys Inc.) and/or SYBYL® (Tripos, Inc.) and/or a docking computer

program such as GOLD (commercially available *via* Cambridge Crystallographic Data Centre, Cambridge, UK; Jones, G., *J. Mol. Biol. 245:* 43-53 (1995)), FlexX (Tripos, Inc.), GRAMM (Ilya A. Vakser, Rockefeller Univ.), Flexidock (Tripos, Inc.), Dock (Ewing, T.J.A. *et al., J. Comput.-Aided Mol. Des. 15:* 411-428 (2001)), or AutoDock (Molecular Graphics Laboratory (Scripps Research Inst.); Goodsell, D.S., *J. Mol. Recognit. 9:* 1-5 (1996)). In addition, other related computer programs may be used.

[0261] The potential inhibitory or binding effect of the chemical entity on a MEK1, MEK2, or MEK-like peptide binding pocket may be analyzed prior to its actual synthesis and testing through the use of computer modeling techniques. The "modeling" includes applying an iterative or rational process to individual or multiple potential ligands, or fragments thereof, to evaluate their association with the MEK1, MEK2, or MEK-like binding pocket and to evaluate their inhibition and/or enhancement of MEK1 or MEK2 activity. This procedure may include, for example, computer fitting a potential ligand into a MEK1, MEK2, or MEK-like peptide binding site(s) to ascertain how well the shape and chemical structure of the potential ligand complements or interferes with the peptide. Computer programs, such as, for example, the program GOLD®, may also be used to estimate the attraction, repulsion and steric hindrance of the ligand to the MEK1, MEK2, or MEK-like binding sites. Generally, the tighter the fit, e.g., the lower the steric hindrance and/or the greater the attractive force, the more antagonistic or agonistic the potential ligand will be since these properties are consistent with a tighter-binding constant. If the theoretical structure, i.e., computational structure, indicates insufficient interaction and association, further testing may not be necessary. However, if computer modeling indicates a strong interaction, then the ligand may be synthesized and tested for its ability to bind to a MEK1, MEK2, or MEK-like binding site(s). Thus, a potential inhibitor or enhancer may be identified and selected, based on its computational ability to positively associate with the amino acid residues found within any one or all of the binding sites.

[0262] Suitable computer programs to be used for computer modeling include, but are not limited to, QUANTA®, CharmM®, INSIGHT®, SYBYL®, MacroModel® and ICM (Dunbrack *et al.*, 1997, supra). SYBYL® may be preferably used. The computer program may be used alone or combined with a docking computer program such as GRAM®, FlexX®, Flexidock®, GOLD® or AUTO DOCK [Dunbrack *et al.*, 1997, supra]. For this purpose, GOLD® may be preferably used.

[0263] The screening method and subsequent identification of potential ligands, may be accomplished *in vivo, in vitro* or *ex vivo.* Initial ligand computation analysis is optional. Instead, or additionally, high-throughput screening may be employed which may be capable of full automation at robotic workstations such that large collections of compound libraries may be screened.

[0264] In one embodiment of the screening and identification method, the initial computer modeling is performed with one or more of the following docking computer modeling programs: Dock (Ewing, T.J.A. *et al., J. Comput.-Aided Mol. Des. 15:* 411-428 (2001)), AutoDock (Molecular Graphics Laboratory; Goodsell, D.S., *J. Mol. Recognit. 9:* 1-5 (1996)), GOLD (commercially available *via* Cambridge Crystallographic Data Centre, Cambridge, UK; Jones, G., *J. Mol. Biol. 245:* 43-53 (1995)) or FlexX (Tripos, Inc.). Potential ligands initially identified by the docking program(s) are elaborated using standard modeling methods as found in, for example, SYBYL® (Tripos, Inc.), QUANTA (Accelrys Inc.), INSIGHT®-II (Accelrys Inc.), GRIN/GRID (Molecular Discovery Ltd.), UNITY® (Tripos, Inc.), LigBuilder (Want, R., *J. Mol. Model 6:* 498-516 (2000)), or SPROUT (developed and distributed by ICAMS (Institute for Computer Applications in Molecular Sciences) at the University of Leeds, United Kingdom (Gillet, V. *et al., J. Comput. Aided Mol. Design 7:* 127-153 (1993))).

[0265] After a potential activity inhibitor and/or enhancer is identified, it can either be selected from commercial libraries of compounds or alternatively the potential inhibitor and/or enhancer may be synthesized and assayed to determine its effect(s) on the activity of MEK1, MEK2, or a structurally related peptide. Optionally, the assay may be radioactive. However, in a preferred embodiment, the assay is a nonradioactive ELISA.

[0266] In one embodiment of screening and identifying potential ligands *via* computer modeling, the method comprises: (a) generating a three-dimensional representation of MEK1 peptide, MEK2 peptide, a structurally related peptide or a MEK-1, MEK-2 or MEK-like peptide binding pocket; (b) designing and/or building (e.g. computationally) *de novo* potential ligands; and (b) identifying the ligands that associate with the MEK1, MEK2, or MEK-like binding site(s). Such ligands may be identified by, for example, contacting the ligand with a cell that expresses MEK1 or MEK2. A MEK1 or MEK2 inhibitor may be identified, for example, as a compound that inhibits the MEK1 or MEK2 catalyzed phosphorylation of ERK1 in the cell. The cell may be a eukaryotic cell, including, but not limited to, a yeast cell or vertebrate. Preferably, the cell is a mammalian cell. More preferably, the cell is a human cell. The protein assay can be an *in vitro, in situ* or *in vivo,* but is preferably an *in vitro* assay. In one such embodiment, the MEK1 or MEK2 catalyzed phosphorylation of ERK1 may be determined by Western blot analysis of ERK di-phosphorylation with ERK phospho-specific antibodies as a direct read-out of MEK activity in the cell. The inhibitory activity of MEK1 or MEK2 ligands may also be screened by *in vitro, ex vivo* or *in vivo* assays. In another embodiment, the assay is performed using a glutathione-S-transferase fusion protein of kinase-inactive ERK1 (GSTERK1K71R) as substrate.

[0267] In an alternative embodiment of screening and identifying potential ligands *via* computer modeling, the method comprises: (a) generating a three-dimensional representation of MEK1, MEK2, a structurally related peptide or a MEK-

1, MEK-2 or MEK-like peptide binding pocket; (b) building (e.g. computationally) and, optionally, modifying, known potential ligands; and (c) identifying the ligands that associate with the MEK-1, MEK-2 or MEK-like peptide binding pocket binding site(s).

[0268] In an alternative embodiment, the compound screening and identification method comprises evaluating the ability of *de novo* compounds to function as MEK1 or MEK2 activity inhibitors and/or enhancers by, for example: (a) generating a MEK1, MEK2, or MEK-like virtual binding cavity, the binding cavity defined by the binding sites; (b) designing (e.g. computationally) a compound structure that spatially conforms to the binding cavity; (c) synthesizing the compound and, optionally, analogs thereof, and (d) testing to determine whether the compound binds to at least one of the binding sites.

[0269] In an alternative embodiment, the compound screening and identification method comprises evaluating the ability of known compounds to function as MEK1 or MEK2 activity inhibitors and/or enhancers by, for example: (a) generating a MEK1, MEK2, or MEK-like virtual binding cavity defined by the binding sites; (b) generating (e.g. computationally) and, optionally, modifying, a known compound structure; (c) determining whether that compound spatially conforms to the binding cavity; (d) synthesizing the compound and, optionally, analogs thereof; and (e) testing to determine whether the compound binds to at least one of the binding sites by.

[0270] In another embodiment, wherein a potential ligand has been selected, the identification method comprises: (a) generating a three-dimensional representation of MEK1, MEK2, or a structurally related peptide with the potential ligand bound thereto; (b) modifying the potential ligand based on the three-dimensional representation; and (c) generating a second three-dimensional representation with the modified potential ligand bound thereto. Then, one can test the potential ligand in a biochemical assay known in the art, if desired.

[0271] In addition, when a potential ligand is identified, a supplemental crystal may be grown comprising the ligand in complex with MEK1, MEK2, or a structurally related peptide, and optionally a cofactor. Molecular replacement analysis, for example, may be used to determine the three-dimensional structure of the supplemental crystal. Molecular replacement analysis may also be used in the initial crystal structure determination.

[0272] It should be understood that in all of the structure-based drug design strategies provided herein, a number of iterative cycles of any or all of the steps may be performed to optimize the selection.

[0273] Thus, according to another embodiment, the invention provides compounds that associate with a MEK1, MEK2 and MEK-like peptide binding pocket(s) produced or identified by any one or a combination of the methods set forth above.

MEK1 and MEK2 Variants

[0274] As mentioned above, the present invention also provides and enables obvious variants of the amino acid sequence of the proteins of the present invention, such as naturally occurring mature forms of the proteins, allelic/sequence variants of the proteins, non-naturally occurring recombinantly derived variants of the proteins, and orthologs and paralogs of the proteins. Such variants can be generated using techniques that are known by those skilled in the fields of recombinant nucleic acid technology and protein biochemistry. It is understood, however, that variants exclude any proteins or peptides disclosed prior to the invention.

[0275] Such variants can readily be identified/made using molecular techniques and the sequence information disclosed herein. Further, such variants can readily be distinguished from other proteins based on sequence and/or structural homology to the proteins of the present invention. The degree of homology/identity present will be based primarily on whether the peptide is a functional variant or non-functional variant, the amount of divergence present in the paralog family, and the evolutionary distance between the orthologs. An alternative method to using the primary sequence for describing the structural relationship between two proteins or peptides is to use the three-dimensional structures of the two related proteins. In this method, the two structures are solved by X-ray crystallography or by NMR, and then the similarity is determined by comparing the root mean square (RMS) deviation of the backbone C-alpha trace of the two species.

[0276] To determine the percent identity of two amino acid sequences or two nucleic acid sequences, the sequences are aligned for optimal comparison purposes (e.g., gaps can be introduced in one or both of a first and a second amino acid or nucleic acid sequence for optimal alignment and non-homologous sequences can be disregarded for comparison purposes). In one aspect of the invention, the length of a reference sequence aligned for comparison purposes is at least 30%, preferably 40%, more preferably 50%, even more preferably 60%. In one preferred embodiment, it is preferably at least 70%, more preferably 80%, or most preferably 90% or more of the length of the reference sequence. The amino acid residues or nucleotides at corresponding amino acid positions or nucleotide positions are then compared. When a position in the first sequence is occupied by the same amino acid residue or nucleotide as the corresponding position in the second sequence, then the molecules are identical at that position (as used herein amino acid or nucleic acid 'identity' is equivalent to amino acid or nucleic acid 'homology'). The percent identity between the two sequences is a function of the number of identical positions shared by the sequences, taking into account the number

of gaps, and the length of each gap, which need to be introduced for optimal alignment of the two sequences.

[0277] The comparison of sequences and determination of percent identity and similarity between two sequences can be accomplished using a mathematical algorithm. (*Computational Molecular Biology,* Lesk, A.M., ed., Oxford University Press, New York, 1988; *Biocomputing: Informatics and Genome Projects,* Smith, D.W., ed., Academic Press, New York, 1993; *Computer Analysis of Sequence Data, Part 1,* Griffin, A.M., and Griffin, H.G., eds., Humana Press, New Jersey, 1994; *Sequence Analysis in Molecular Biology,* von Heinje, G., Academic Press, 1987; and *Sequence Analysis Primer,* Gribskov, M. and Devereux, J., eds., M Stockton Press, New York, 1991). In a preferred embodiment, the percent identity between two amino acid sequences is determined using the Needleman and Wunsch (*J. Mol. Biol.* (48): 444-453 (1970)) algorithm which has been incorporated into commercially available computer programs, such as GAP in the GCG software package, using either a Blossom 62 matrix or a PAM250 matrix, and a gap weight of 16, 14, 12, 10, 8, 6, or 4 and a length weight of 1, 2, 3, 4, 5, or 6. In yet another preferred embodiment, the percent identity between two nucleotide sequences can be determined using the commercially available computer programs including the GAP program in the GCG software package (Devereux, J., *et al., Nucleic Acids Res. 12(1)*: 387 (1984)), the NWS gap DNA CMP matrix and a gap weight of 40, 50, 60, 70, or 80 and a length weight of 1, 2, 3, 4, 5, or 6. In another embodiment, the percent identity between two amino acid or nucleotide sequences is determined using the algorithm of E. Meyers and W. Miller (CABIOS, 4: 11-17 (1989)) which has been incorporated into commercially available computer programs, such as ALIGN (version 2.0), using a PAM120 weight residue table, a gap length penalty of 12 and a gap penalty of 4.

[0278] The nucleic acid and protein sequences of the present invention can further be used as a "query sequence" to perform a search against sequence databases to, for example, identify other family members or related sequences. Such searches can be performed using commercially available search engines, such as the BLASTN and BLASTX programs (version 2.0) of Altschul, *et al.* (*J. Mol. Biol.* 215: 403-10 (1990)). BLAST nucleotide searches can be performed with the BLASTN program, score = 100, wordlength = 12 to obtain nucleotide sequences homologous to the nucleic acid molecules of the invention. BLAST protein searches can be performed with the BLASTX program, score = 50, wordlength = 3 to obtain amino acid sequences homologous to the proteins of the invention. To obtain gapped alignments for comparison purposes, Gapped BLAST can be utilized as described in Altschul *et al.* (*Nucleic Acids Res.* 25(17): 3389-3402 (1997)). When utilizing BLAST programs, the default parameters of the respective programs (e.g., BLASTX and BLASTN) can be used.

[0279] Full-length clones comprising one of the proteins of the present invention can readily be identified as having complete sequence identity to one of the kinases of the present invention as well as being encoded by the same genetic locus as the MEK1 or MEK2 peptide provided herein.

[0280] Allelic variants of a peptide can readily be identified as having a high degree (significant) of sequence homology/identity to at least a portion of the protein as well as being encoded by the same genetic locus as the MEK1 or MEK2 peptide provided herein. As used herein, two proteins (or a region of the proteins) have significant homology when the amino acid sequences are typically at least 70%, preferably 75%, more preferably 80%, or even more preferably 85% or more homologous. In one preferred embodiment, it is at least 90%, or preferably 95% or more homologous. A significantly homologous amino acid sequence, according to the present invention, will be encoded by a nucleic acid sequence that will hybridize to a protein encoding nucleic acid molecule under stringent conditions as more fully described below.

[0281] Paralogs of a protein can readily be identified as having some degree of significant sequence homology/identity to at least a portion of the MEK1 or MEK2 peptide, as being encoded by a gene from same species, and as having similar activity or function. Two proteins will typically be considered paralogs when the amino acid sequences are typically at least 70%, preferably 75%, more preferably 80%, even more preferably 85% or more homologous through a given region or domain. In one preferred embodiment, two proteins will typically be considered paralogs when the amino acid sequences are typically 90% or more, preferably 95% or more homologous through a given region or domain. Such paralogs will be encoded by a nucleic acid sequence that will hybridize to a kinase peptide encoding nucleic acid molecule under stringent conditions as more fully described below. An example of a paralog is the relationship between MEK2 and MEK1. These proteins are 80% homologous overall, 85% homologous in the kinase domain and 100% homologous in the ATP- and ligand-binding domain. In addition, as MEK2 is inhibited by the MEK1 inhibitors, and as the active sites have been found to be identical, the three-dimensional structure or X-ray crystallographic coordinates of the MEK1 peptide may be used to identify MEK2 inhibitors. Conversely, the three-dimensional structure or X-ray crystallographic coordinates of the MEK2 peptide may be used to identify MEK1 inhibitors.

[0282] Orthologs of a protein can readily be identified as having some degree of significant sequence homology/identity to at least a portion of the protein as well as being encoded by a gene from another organism. Preferred orthologs will be isolated from mammals, preferably human, for the development of human therapeutic targets and agents, or other invertebrates, particularly insects of economical/agriculture importance, e.g. members of the Lepidopteran and Coleopteran orders, for the development of insecticides and insecticidal targets. Such orthologs will be encoded by a nucleic acid sequence that will hybridize to a MEK1 or MEK2 encoding nucleic acid molecule under

moderate to stringent conditions, as more described below, depending on the degree of relatedness of the two organisms yielding the proteins.

[0283] Non-naturally occurring variants of the MEK1 or MEK2 peptide of the present invention can readily be generated using recombinant techniques. Such variants include, but are not limited to deletions, additions and substitutions in the amino acid sequence of the protein. For example, one class of substitutions is conserved amino acid substitution. Such substitutions are those that substitute a given amino acid in a protein by another amino acid of like characteristics. Typically seen as conservative substitutions are the replacements, one for another, among the aliphatic amino acids Ala, Val, Leu, and Ile; interchange of the hydroxyl residues Ser and Thr; exchange of the acidic residues Asp and Glu; substitution between the amide residues Asn and Gln; exchange of the basic residues Lys and Arg; and replacements among the aromatic residues Phe, Tyr. Guidance concerning which amino acid changes are likely to be phenotypically silent are found in Bowie *et al., Science 247*:1306-1310 (1990).

[0284] Variants can be fully functional or can lack function in one or more activities. Fully functional variants typically contain only conservative variation or variation in non-critical residues or in non-critical regions. Functional variants can also contain substitution of similar amino acids, which result in no change or an insignificant change in function. Alternatively, such substitutions may positively or negatively affect function to some degree.

[0285] Amino acids that are essential for function can be identified by methods known in the art, such as site-directed mutagenesis or alanine-scanning mutagenesis (Cunningham *et al., Science 244*:1081-1085 (1989)). The latter procedure introduces single alanine mutations at every residue in the molecule. The resulting mutant molecules are then tested for biological activity such as receptor binding or *in vitro* proliferative activity. Sites that are critical for binding can also be determined by structural analysis such as X-ray crystallography, nuclear magnetic resonance or photoaffinity labeling (Smith *et al., J. Mol. Biol. 224*:899-904 (1992); de Vos *et al. Science 255*:306-312 (1992)).

[0286] The following examples illustrate preferred embodiments and aspects of the invention, and are intended to be non-limiting.

EXAMPLES

Example 1: Cloning of modified MEK1s

[0287] Human MEK1 cDNA (GenBank Accession Number L11284; SEQ ID NO: 1) was modified via PCR and subcloned into pET24b (Novagen) at 5'*Nde1*/3'*HindIII* sites. Wild type MEK1 was modified via PCR for cloning into pET21b and pET24b expression vectors by the addition of 5'NdeI and 3'HindIII restriction sites with the following oligonucleotides:

5'CATATGCCGAAAAAGAAGCCGACCCCGATCCAG3' (SEQ ID NO: 5)

5'AAGCTTGACGCCAGCAGCATGGGTT3' (SEQ ID NO: 6)

[0288] Conditions for PCR were as follows: 20ng MEK DNA, 20pmoles of both 5' and 3' primers, 200μM dNTP mix, 1X PCR 10X Vent buffer, 1 unit Vent DNA polymerase in a reaction volume of 100μl. Reactions were run at 95°C for 5 min (1 cycle), followed by 25 cycles of 95°C 1 min, 56°C 1 min, 72°C for 1 min 30 sec. Wild-type MEK1 ("MEK1(wt)") sequence was altered on the region spanning from bp 73 to bp 99 for tRNA bias in *E. coli,* with the following base changes, highlighted in bold and underlined: 5'ATGCC**G**AA**A** AAGAAGCCGAC**C**CC**G**ATC3' (amino acid residues 73-99 of SEQ ID NO: 2). A NH_2-terminally truncation of MEK1 was also generated by PCR, designated C1 ("MEK1-C1"), encoding amino acids 51-393 of SEQ ID NO: 2. The MEK1-C1 clone was subcloned into pET21b (Novagen, Madison, WI) at the 5'*Nde1*/3'*Xho1* sites. Additionally, both MEK1 (wt) and MEK1-C 1 clones were modified by deletion of a proline-rich insertion loop, comprised of residues 280-323 to give MEK1 (wt)(d280-323) and MEK1-C1 (d280-323), respectively. This deletion was created by introducing an internal *HindIII* site which encoded residues 324 and 325 with the following sequence: AAG(K280)CTT(L323). Fragment A, containing the coding sequence NH_2-terminally to the deletion (amino acids 1-279 for MEK1 (wt), and residues 51-279 for the MEK1-C1), was modified by PCR to contain a *HindIII* site on the 3' end downstream of amino acid 279 (V). This fragment was then ligated to fragment B, a 0.2kb fragment containing sequence for residues 324-393, including the codon changes for amino acids 324 and 325 to become a *HindIII* site. Both MEK1 (wt)(d280-323) and MEK1-C1 (d280-323) clones were subcloned into pET24b (Novagen, Madison, WI) at 5'*Nde1*/3'*Xho1* sites. All modified MEK cDNA sequences were verified using MEK1-specific sequencing primers in an automated sequencing apparatus (ABI technologies). Once a nucleotide sequence was obtained, it was compared to the deposited sequence for MEK1 to confirm sequence integrity.

[0289] By following a similar procedure, the following NH_2-terminally truncated MEK1 peptides were prepared:

MEK1-C2: NH_2-terminally truncated MEK1 having peptide of amino acid residues 62 to 393 of the sequence of SEQ ID NO: 2.
MEK1-C2 (d280-323): MEK1-C2 having a deletion from amino acid residues from 280 to 323 of the sequence of SEQ ID NO: 2.
MEK1-C3: NH_2-terminally truncated MEK1 having peptide of amino acid residues 42 to 393 of the sequence of SEQ ID NO: 2.
MEK1-C3 (d280-323): MEK1-C3 having a deletion from amino acid residues from 280 to 323 of the sequence of SEQ ID NO: 2.
MEK1 (d280-323): MEK1 having a deletion from amino acid residues from 280 to 323 of the SEQ ID NO: 2.
MEK1 (d264-310): MEK1 having a deletion from amino acid residues from 264 to 310 of the SEQ ID NO: 2.
MEK1 (d270-310): MEK1 having a deletion from amino acid residues from 270 to 310 of the SEQ ID NO: 2.
MEK1 (d264-305): MEK1 having a deletion from amino acid residues from 264 to 305 of the SEQ ID NO: 2.
MEK1 (d267-307): MEK1 having a deletion from amino acid residues from 267 to 307 of the SEQ ID NO: 2.
MEK1 (d265-304): ME The software may be used to add hydrogens to the PDB molecular structure file in standardized geometry with optimization of orientations of OH, SH, NH_3^+, Met methyls, Asn and Gln sidechain amides, and His rings.K1 having a deletion from amino acid residues from 265 to 304 of the SEQ ID NO: 2.

[0290] The following primers were used for PCR of the modified MEK1s.

MEK1-C1 and MEK1-C1 (d280-323):

For fragment A: 5' CTTGCATATG GAGGCCTTTC TTACCCAGA 3' (SEQ ID NO: 7)

For fragment B: 5' CTTGAAGCTT CACCTGGCAC CCAAACATC 3' (SEQ ID NO: 8)

MEK1-C2 and MEK1-C2 (d280-323):

For fragment A: 5' CTTGCATATG GAACTGAAGG ATGACGACTT 3' (SEQ ID NO: 9)

For fragment B: 5' CTTGAAGCTT CACCTGGCAC CCAAACATC 3' (SEQ ID NO: 8)

MEK1-C3 and MEK1-C3 (d280-323):

For fragment A: 5' CTTGCATATG CTTGATGAGC AGCAGCGAA 3' (SEQ ID NO: 10)

For fragment B: 5' CTTGAAGCTT CACCTGGCAC CCAAACATC 3' (SEQ ID NO: 8)

Example 2: Cloning of modified MEK2s

[0291] Human MEK2 cDNA (GenBank Accession Number NM_030662; SEQ ID NO: 3) was modified via PCR and subcloned into pET24b (Novagen) at 5'Nde1/3'HindIII sites. Wild type MEK2 was modified via PCR for cloning into pET24b expression vectors by the addition of 5'Nde1 and 3'HindIII restriction sites with the following oligonucleotides:

5'CATATG AAGCCGGTGCTGCCGGCGCTCACCATC3' (SEQ ID NO: 11) 5'AAGCTTGGCCACTGTCACACGGCGGTG3' (SEQ ID NO: 12)

[0292] Conditions for PCR were as follows: 20ng MEK DNA, 20pmoles of both 5' and 3' primers, 200μM dNTP mix, 1X PCR 10X Vent buffer, 1 unit Vent DNA polymerase in a reaction volume of 100μl. Reactions were run at 95°C for 5 min (1 cycle), followed by 25 cycles of 95°C 1 min, 56°C 1 min, 72°C for 1 min 30 sec.

[0293] Six N-termina truncations of wild type human MEK2 cDNA were generated via PCR amplification and cloned into pET201 TA-TOPO vector (Invitrogen). Each is fused with a C-terminal His6 tag.

[0294] Sequencing of the template DNA pET24b MEK2 wild type revealed a silent mutation on amino acid residual V64: GTC to GTT.

[0295] Conditions for PCR were as follows: pET24b MEK2 wild type DNA 1ng/ul, 5' and 3' primers 1 μM, 1x Pfx Amplification Buffer, 0.3 mM dNTP mixture, 5 unit Platinum Pfx DNA polymerase in a reaction volume of 100μl. Reactions were run at 94°C for 3 min (1 cycle), followed by 35 cycles of 94°C 1 min, 55°C 30 seconds, 68°C 1 min 30 sec, followed by 1 cycle of 68°C 10 min. The 3' A overhangs of the PCR products were added by 1 cycle of 68°C 10 min in the above PCR mixture plus 0.1 mM dATP and 2.5 unit of Taq DNA Polymerase.

[0296] Six varied NH_2-terminal truncations were used in the creation of the modified MEK2 peptides. Each of the six constructs possessed a Hexahistidine tag fused to the COOH-terminal:

MEK2-C1: amino acid residues 46 to 400 of the sequence of SEQ ID NO:3;
MEK2-C2: amino acid residues 55 to 400 of the sequence of SEQ ID NO:3;
MEK2-C3: amino acid residues 66 to 400 of the sequence of SEQ ID NO:3;
MEK2-C4: amino acid residues 59 to 400 of the sequence of SEQ ID NO:3;
MEK2-C5: amino acid residues 62 to 400 of the sequence of SEQ ID NO:3;
MEK2-C6: amino acid residues 64 to 400 of the sequence of SEQ ID NO:3;

[0297] The following primers were used for PCR generation of the MEK2 N-terminal truncations:

MEK2-C1: forward primer: 5' ATGCTTGACGAGCAGCAGAAGAAG 3' (SEQ ID NO: 13)

MEK2-C2: forward primer: 5' ATGGAAGCCTTTCTCACCCAGAAAGCC 3' (SEQ ID NO: 14)

MEK2-C3: forward primer: 5' ATGGCCTTTCTCACCCAGAAAGCC 3' (SEQ ID NO: 15)

MEK2-C4: forward primer: 5' ATGACCCAGAAAGCCAAGGTTGG 3' (SEQ ID NO: 16)

MEK2-C5: forward primer: 5' ATGGCCAAGGTCGGCGAACTCAAAGAC 3' (SEQ ID NO: 17)

MEK2-C6: forward primer: 5' ATGGTCGGCGAACTCAAAGACGATGAC 3' (SEQ ID NO: 18)

[0298] The common reverse primer for all the above six MEK2 trunctions:

5' TCAATGATGATGATGATGTTCAAGCACAGCGGTGCGCGTGGGTG 3' (SEQ ID NO: 19)

[0299] Sequences for the above six MEK2 truncations were verified using pET201 vector sequencing primers (T7 promoter and T7 Terminator primers) in an automated sequencing apparatus (ABI technologies). Once a nucleotide sequence was obtained, it was compared to the deposited sequence for MEK2 to confirm sequence integrity.

Example 3: Large scale expression of the modified MEK1s in *E. coli*

[0300] The recombinant MEK1 constructs obtained from Example 1 were grown at 37°C in *E. coli* BL21 (DE3) in a 10-liter fermentor containing rich media. A starter culture of Kanamycin resistant MEK1 was grown by inoculating a 1 L shake flask of LB media with 100 μL of glycerol stock. The culture was grown overnight at 30°C in a shaking incubator set to 250 rpm. The next morning the entire liter of culture was added to a 10-liter fermentor containing rich media prepared using the recipe (260.0 g yeast extract (Difco 0127), 260.0 g BBL Acidicase peptone, 260.0 g casitone (Difco 0259) dissolved in distilled water to 4.0 L. Add 260.0 g dry gelatone (Difco 0657) then 26.0 g KH_2PO_4 anhydrous, 26.0 g K_2HPO_4 anhydrous, 26.0 g $Na_2HPO_4.7H_2O$, dissolved with distilled water to 2.0 L and added 0.5% (v/v) glycerol) or Super Broth (KD Medical, Columbia, MD). At an optical density at 600nm of 10, the temperature was decreased to 22-25°C for one hour and recombinant protein expression was induced by addition of IPTG (isopropylthio-beta-D-galactoside) to a concentration of 1.0 mM. For the Rich media preparation without glycerol supplementation the fermentor was harvested eighteen hours after induction. For the Super Broth preparation or the Rich media preparation with glycerol supplementation the fermentor was harvested thirty-six hours after induction. A typical yield was about 700g whole cells / 10 L fermentation.

[0301] The cell pellet was resuspended 1:5 (w/v) in 50mM K_2HPO_4, 2mM TCEP (Tri(2-carboxyethyl)phosphine), 300mM NaCl, 5 mM $MgCl_2$, 10mM CHAPS (3-([3-cholamidopropyl]dimethylammonio)-1-propanesulfonate), at pH 8.0. Cell disruption was carried out using a Dyno-Mill KDL. Fifty μL of Benzonase (EM Industries, Hawthorne, NY) was included during lysis. The lysis was clarified by centrifugation for 45 minutes at 13,600 times g at 4°C.

Example 4: Large scale expression of the modified MEK2s in E. coli

[0302] The recombinant MEK2 constructs obtained from Example 2 were grown at 37°C in *E. coli* BL21 (DE3) in a 10-liter fermentor containing rich media. A starter culture of Kanamycin resistant MEK1 was grown by inoculating a 1 L shake flask of LB media with 100 μL of glycerol stock. The culture was grown overnight at 30°C in a shaking incubator set to 250 rpm. The next morning the entire liter of culture was added to a 10-liter fermentor containing rich media prepared using the recipe (260.0 g yeast extract (Difco 0127), 260.0 g BBL Acidicase peptone, 260.0 g casitone (Difco 0259) dissolved in distilled water to 4.0 L. Add 260.0 g dry gelatone (Difco 0657) then 26.0 g KH_2PO_4 anhydrous, 26.0 g K_2HPO_4 anhydrous, 26.0 g $Na_2HPO_4.7H_2O$, dissolved with distilled water to 2.0 L and added 0.5% (v/v) glycerol) or Super Broth (KD Medical, Columbia, MD). At an optical density at 600nm of 10, the temperature was decreased to

22-25°C for one hour and recombinant protein expression was induced by addition of IPTG (isopropylthio-beta-D-galactoside) to a concentration of 1.0 mM. For the Rich media preparation without glycerol supplementation the fermentor was harvested eighteen hours after induction. For the Super Broth preparation or the Rich media preparation with glycerol supplementation the fermentor was harvested thirty-six hours after induction. A typical yield was about 700g whole cells / 10 L fermentation.

[0303] The cell pellet was resuspended 1:3 (w/v) in 50mM K_2HPO_4, 2mM TCEP (Tri(2-carboxyethyl)phosphine), 5 mM Imidazole, 300mM NaCl, 5 mM $MgCl_2$, 2mM pyrrole-2-carboxylate and 100μM $ZnCl_2$, 10mM CHAPS (3-([3-cholamidopropyl]dimethylammonio)-1-propanesulfonate), at pH 8.0. Cell disruption was carried out using a Dyno-Mill KDL. Fifty μL of Benzonase (EM Industries, Hawthorne, NY) was included during lysis. The lysis was clarified by centrifugation for 45 minutes at 13,600 times g at 4°C.

Example 5: Purification of modified MEK1s

[0304] The cell lysate was mixed 1:1 with 2X binding buffer (50mM K_2HPO_4, 10mM imidazole, 4mM TCEP, 300mM NaCl, 10mM CHAPS, 2mM pyrrole-2-carboxylate and 100μM $ZnCl_2$, pH=8.0) and combined with washed TALON™ metal affinity resin (ClonTech, Cat # 8908-2) at a ratio of 2mL of resin per 1g of cells. The mixture was stirred at 4°C for 1 hour, then batch-loaded into a 5-L Amicon (Vantage-S) column. Any additional unbound proteins/impurities were eluted with the washing buffer (50mM K_2HPO_4, 5mM imidazole, 2mM TCEP, pH 8.0 and 300mM NaCl, 1mM pyrrole-2-carboxylate, 50μM $ZnCl_2$) until a baseline reading was reached. The protein was eluted with 4-5 column volumes of elution buffer (20mM HEPES, 100mM EDTA disodium salt, 2mM TCEP, pH 8.0 and 10%v/v glycerol) and concentrated 10-fold using a Millipore (S1Y10) spiral cartridge. The protein concentrate was then diluted 10-fold in HS buffer A (20mM MES (2-(N-morpholino)-ethanesulfonic acid), 2mM TCEP, pH 6.4 and 20% ethylene glycol) and loaded onto a pre-equilibrated HS column (POROS HS/20 25X100, Applied Biosystems). The protein was eluted with a linear gradient from 0-100% HS Buffer B (Buffer A and 1M ammonium acetate). The protein containing fractions were pooled together and concentrated using a Millipore ultrafiltration stir-cell (YM10 membrane). The protein concentrate was then diluted 50X in HQ Buffer A (20mM TRIS Tris(hydroxymethyl) aminomethane), 2mM TCEP, pH 8.0 and 10mM ammonium acetate) and loaded on to a pre-equilibrated HQ column (POROS HQ/20 16X100, Applied Biosystems). The protein was eluted in the unbound fraction and was immediately concentrated using a Millipore ultrafiltration stir-cell (YM10 membrane). The protein:inhibitor complexes were purified by adding a 10-fold molar excess of the inhibitor was and stirring overnight at 4°C. The sample was then filtered using a 0.22μm polyethersulfone filter, further concentrated using a YM10 membrane fitted stir-cell, centrifuged at 8000 rpm for 30 minutes at 4°C, and loaded onto a pre-equilibrated size exclusion column (HiLoad 26/60 Superdex 200 prep grade, Pharmacia, # 17-1071-01). The protein was eluted in approximately 5 hours using the size exclusion chromatography buffer (20mM HEPES, 0.5mM EDTA disodium salt, 2mM TCEP, pH 7.5 and 150 ammonium acetate and 50nM inhibitor). The inhibitor used to form the ternary complex was 5-bromo-N-(2,3-dihydroxy-propoxy)-3,4-difluoro-2-(2-fluoro-4-iodo-phenylamino)-benzamide. The protein-containing fractions were pooled together, concentrated using a Millipore ultrafiltration stir-cell (YM10 membrane), centrifuged at 14,000 rpm for 10 minutes at 4°C, aliquoted into microcentrifuge tubes, and snap-frozen in liquid nitrogen. The protein aliquots were stored at -80°C until needed for crystallization. The same procedure was followed for the purification of the apo protein except that the concentrated HQ flow-through was loaded directly onto the pre-equilibrated size exclusion column.

Example 6: Purification of modified MEK2s

[0305] The cell lysate was combined with washed TALON™ metal affinity resin (ClonTech, Cat # 8908-2) at a ratio of 1mL of resin per 5g of cells. The mixture was stirred at 4°C for 1 hour, then batch-loaded into a Biorad Econo column. Any additional unbound proteins/impurities were eluted with the washing buffer (50mM K_2HPO_4, 5mM imidazole, 2mM TCEP, pH 8.0 and 300mM NaCl, 1mM pyrrole-2-carboxylate, 50μM $ZnCl_2$) until a baseline reading was reached. The protein was eluted with 4-5 column volumes of elution buffer (20mM HEPES, 100mM EDTA disodium salt, 2mM TCEP, pH 7.5 and 10%v/v glycerol). The eluted protein was then diluted 10-fold in HS buffer A (20mM MES (2-(N-morpholino)-ethanesulfonic acid), 2mM TCEP, pH 6.4 and 20% ethylene glycol) and loaded onto a pre-equilibrated HS column (POROS HS/20 25X100, Applied Biosystems). The protein was eluted with a linear gradient from 0-100% HS Buffer B (Buffer A and 1M ammonium acetate. The protein containing fractions were pooled together and concentrated using a Millipore ultrafiltration stir-cell (YM10 membrane). The protein concentrate was then loaded onto a pre-equilibrated size exclusion column (HiLoad 26/60 Superdex 200 prep grade, Pharmacia, # 17-1071-01). The protein was eluted in approximately 5 hours using SEC buffer (20mM HEPES, 0.1mM EDTA disodium salt, 2mM TCEP, pH 7.5 and 150 ammonium acetate). The protein containing fractions were pooled and protein:ligand complex was formed by adding 10-fold molar excess of the ligand, {5-[3,4-Difluoro-2-(2-fluoro-4-iodo-phenylamino)-phenyl]-1,3,4-oxadiazol-2-yl}-(2-morpholin-4-yl-ethyl)-amine (dissolved in DMSO), dropwise into the protein solution under constant stirring. After

stirring overnight at 4°C, the complex was concentrated using a YM10 membrane fitted stir-cell, centrifuged at 8000 rpm for 30 minutes at 4°C, aliquoted into microcentrifuge tubes, and snap-frozen in liquid nitrogen. The protein aliquots were stored at -80°C until needed for crystallization.

Example 7: *In vivo* and *in vitro* MEK1 and MEK2 activity assays

[0306] The kinase activity of the modified MEK1 peptides was assayed using a glutathione-S-transferase fusion protein of kinase-inactive ERK1 (GSTERK1K71R) as substrate. The modified MEK peptides (50ng) were assayed in 20mM HEPES (N-2-hydroxyethyl-piperazine-N'-2-ethanesulfonic acid) pH 7.5, 10mM $MgCl_2$, 1mM EGTA (ethylene glycol bis(2-aminoethyl ether)-N,N,N'N'-tetraacetic acid), 10μM ATP, with 5μCi [γ-^{32}P] ATP. Appropriate samples had 0.5 units of Raf-1 (UBI) added, and the reaction started with the addition of 1 μg GSTERK1 (K71R). The reactions were incubated at room temperature for 20 minutes, then quenched with 5μl 6x Laemmli sample buffer. The samples were then resolved by SDS-PAGE, and the phosphoproteins visualized by autoradiography. Radiolabel incorporated into ERK was quantitated by excision of the protein band from the gel and counting in a standard scintillation counter. Initial experiments with the modified MEK1s generated the following specific activities in units of pmol PO4 min-1 mg-1 after Raf activation: WT: 8380.6, W§TPR: 40.1, C1FL: 773.3, C1§PR: 35.9, C2FL: 537.5, C2§PR: 24.1, C3FL: 441.7 and C3§PR: 26.9.

[0307] In the evaluation of ligand that has been designed using the three-dimensional structural information of the MEK1: ligand: cofactor complexes, 5-bromo-N-(2,3-dihydroxy-proxy)-3,4-difluoro-2-(2-fluoro-4-iodo-phenylamino)-benzamide was added to 96 well format plates with filter bottomed wells. Kinase-inactive ERK1 (K71R mutant) in HEPES buffer is then added to each well. After subsequent addition of MEK1 (2D mutant) diluted in a Tris buffer before being added to the plate, and the reaction is initiated by the addition of radioactive ATP, diluted in 0.05% Tween 20. After 1 hour incubation at room temperature, ice-cold 20% TCA is added to each well to stop the reaction and to precipitate the protein in solution. Filtration is done the following day, followed by scintillation counting of the incorporated radioactivity using a Perkin Elmer Wallac microBeta 1450 counter. Inhibition is expressed as a percentage of the vehicle control.

(1) Evaluation of *ex vivo* tissue samples for pMAPK levels

[0308] A lysis buffer of 50mM glycerol phosphate, 10mM HEPES, pH7.4, 1% Triton x-100, 70mM NaCl, 1mM Na_3VO_4, 100μM PMSF, 10μM leupeptin, and 10μM pepstatin. (Only add the inhibitors when ready to use) was prepared. Tumors are removed at -70° and placed onto dry ice immediately. 40-50 mg of each tumor is weighed and sliced using a scalpel. The mixture was homogenized with polytron and centrifuged at 2500 rpm at 4°□ for 15 minutes. A supernatant was transferred to a 15 mL Falcon tube. The protein assay was then run and protein was normalized to about 15μg. 5μL - 10μL of 6X laemmli was added to each tube depending on the amount of lysate. The mixture was boiled for 3 minutes, spin and run on 10% tris-gly gels at 140V (Bio-Rad). Transfer was accomplished at 125V for 1.5 - 2 hours. The membrane was rinsed in water, and was then placed into blocking solution of TBST (Tris-buffered saline-Tween 20), 1%BSA and 1% ovalbumin. The membrane was rinsed three times for 5 minutes in TBST and was then placed into the primary antibody (Promega) for 3-4 hours. The membrane was then washed for 5 minutes in TBST and was placed into the secondary antibody (Bio-Rad Goat anti-rabbit HRP) for 1.5 hours. The blots were visualized by ECL (Pierce). Protein bands, identified as phosphorylated MAPK were measured using densitometry using a Biorad Flur-S Multilmager Max.

(2) *In vivo* Colon26 Cellular MAP Kinase Western Assay:

[0309]

Day 1 Colon26 (murine) cells were seeded in twelve-well plates at roughly $2x10^5$ cells/well (1.5 ml/well). The cells were grown in media consisting of DMEM/F12 #11330-032 (Gibco), 10% FBS and 1% antibiotic/antimycotic and incubated at 37°C, 5% CO_2 overnight.

Day 2 Compounds were prepared in DMSO at concentrations of (1, 0.3, 0.1, 0.03, 0.01, 0.003, and 0.001 μM) in a 96-well plate. The DMSO concentration in the cell preparations should never be greater than 0.2 %; therefore, a total of 3 μl of each DMSO solution was added to a 1.5 ml well containing cells. The cells were then incubated at 37° in a 5% CO_2 incubator for one hour.

[0310] The plates and eppendorf tubes were kept on ice. The cells were washed in 1 ml PBS (containing 1mM Na_3VO_4) followed by removal of PBS. The state of threonine and tyrosine phosphorylation of cellular MAPK was determined after treatment by lysing cells in 100 uLμ of a solution containing 70 mM NaCl, 50 mM glycerol phosphate, 10 mM HEPES, pH 7.4, 1% Triton X-100, 1 mM Na_3VO_4, 100 μM PMSF, 10 μM leupeptin and 10 μM pepstatin. The

cells were scraped from the wells and transferred to an eppendorf tube. The eppendorf tubes were spun at 13,000 rpm at 4 degrees for 5 min. The supernatant was then transferred to cold eppendorf tubes and the pellet was discarded. The Pierce BCA protein assay was then run and proteins were standardized to 20 μg. Either a 10% tris-glycine 10 well or 15 well gel was loaded and the gel was run at 130V for 1.5 hours. Transfer was accomplished at 125V for 2 hours or at 25V overnight. The membrane was rinsed in water, and was then placed into blocking solution for 1-18 hours. The membrane was rinsed three times for 5 minutes in TBST and was then placed into the primary antibody (pMAPK) for 3-18 hours. The membrane was then washed for 5 minutes in TBST and was placed into the secondary antibody (Bio-Rad Goat anti-rabbit HRP) for one hour. The membrane was finally washed three times for 15 minutes in TBST. The blots were visualized by ECL (Pierce). Protein bands, identified as phosphorylated MAPK were measured using densitometry using a Biorad Flur-S MultiImager Max. To evaluate total MAPK levels, blots were subsequently 'stripped' and re-probed with a 1:1 mixture of polyclonal antibodies recognizing unphosphorylated ERK1 and ERK2 (Santa Cruz Biotechnology, Santa Cruz, California).

(3) Materials List:

[0311]

TBST buffer 0.9% NaCl, 10mM Tris, 0.1% Tween-20, pH 7.5
pMAPK Promega pMAPK: (1:5,000 in 0.5% BSA) #V8031-Polyclonal
Secondary BioRad Goat-anti-Rabbit HRP (1:10,000 in 0.5% BSA)
Catalogue # 170-6515
Blocking Solution: 1% BSA, 1%Ovalbumin in TBST, filter sterilized with 0.01% Na Azide

Example 8: Crystallization of the MEK1: ligand: cofactor complexes

[0312] The purified protein: ligand complexes (MEK1-C2, MEK1-C1, MEK1-C1(d280-323)) described in Example 4 were quick-thawed and incubated overnight at 4°C with a cofactor solution consisting of 5 mM Mg-ATP dissolved in the size exclusion chromatography buffer as described above. After incubation, the protein: ligand: cofactor complexes were centrifuged for 30 minutes at 14,000 x g at 4°C. Crystals of the MEK1 C2 peptide: ligand: cofactor complexes were grown by hanging drop vapor diffusion at 13°C using 1 μL drops of the ternary complex, with a protein to precipitant ratio of 1:1 over a 1 mL well solution. The precipitant used was 6-16% (w/v) PEG 8K, 150-450 mM $NH_4H_2PO_4$, 20 mM DTT, and 100 mM imidazole/malate buffer, pH 7.0. The crystals grew to about 0.2 x 0.1 x 0.1 mm in about 8 days.

[0313] Alternatively, 60 μL of the purified apo protein solution described in Example 4 was combined with about 0.2 mg of an inhibitor for a period between 2 - 8 hours. The solution of the MEK1 peptide: ligand complex was then incubated overnight at 4°C with a cofactor solution consisting of 5 mM Mg-ATP dissolved in the size exclusion chromatography buffer and crystallized as described above.

[0314] The crystals were prepared for low temperature data collection by bathing the crystal in a cryoprotectant solution consisting of 10% ethylene glycol diluted with the well solution. The procedure comprises adding a 1 μL drop of the 100% ethylene glycol solution to the inverted coverslip containing the crystal. The cryo solution was then thoroughly mixed with 9μL of the well solution to create a 10% ethylene glycol cryo solution. The mixed cryo solution was then added in a ratio of 1:1 (v/v) to the drop containing the crystal and allowed to slowly mix by diffusion. The drop containing the crystal, called the mother liquor, is now composed of 5% ethylene glycol. After about 2 minutes, the crystal was removed from the cryo/ mother liquor solution and transferred into a mixture of 70% Paratone-N obtained from Hampton Research, Laguna Niguel, CA and 30% light, white mineral oil mixture using a mounted cryo loop, also obtained from Hampton Research, Laguna Niguel, CA. The crystal was then manipulated in the oil mixture to completely remove the aqueous solution and then quickly cooled by immersion directly into liquid nitrogen. Alternatively, the crystals may be dipped in a stream of cold nitrogen gas at about 100 K.

Example 9: Crystallization of the MEK2: ligand: cofactor complexes

[0315] The purified protein: ligand complexes MEK2-C2, described in Example 6 were quick-thawed and incubated overnight at 4°C with a cofactor solution consisting of 5 mM Mg-ATP dissolved in the size exclusion chromatography buffer as described above. After incubation, the protein: ligand: cofactor complexes were centrifuged for 30 minutes at 14,000 x g at 4°C. Crystals of the MEK2 peptide: ligand: cofactor complexes were grown by hanging drop vapor diffusion at 13°C using 1 μL drops of the ternary complex, with a protein to precipitant ratio of 1:1 over a 1 mL well solution. The precipitant used was 1.4-1.85 M NaH_2PO4/ K_2HPO4, 0-20 mM DTT, pH 6.7-7.1. The crystals grew to about 0.2 x 0.1 x 0.1 mm in about 8 days.

[0316] The crystals were prepared for low temperature data collection by bathing the crystal in a cryoprotectant solution consisting of a mixture of 70% Paratone-N obtained from Hampton Research, Laguna Niguel, CA and 30% light, white mineral oil mixture using a mounted cryo loop, also obtained from Hampton Research, Laguna Niguel, CA. The crystal was then manipulated in the oil mixture to completely remove the aqueous solution and then quickly cooled by immersion directly into liquid nitrogen. Alternatively, the crystals may be dipped in a stream of cold nitrogen gas at about 100 K.

Example 10: Crystallographic data collection of the MEK1 and MEK2: ligand: cofactor complex crystals

(1) In-house analysis and collection of diffraction data:

[0317] The initial data set used for phase determination was collected at 100 Kelvin on an R-AXIS IV^{++} mounted on a Rigaku RU-H3R rotating anode X-ray source operating at 50 kV and 100 mA equipped with an Osmic confocal mirror. The detector was positioned at a 2 theta value of 0 degrees with a crystal to detector distance of 225 mm. A rotation angle of 0.5 degree per frame was used with an exposure time of 10 minutes per frame. The inverse-beam method was used with two 80° sweeps collected 180° apart.

(2) Synchrotron data collection:

[0318] Synchrotron data sets of MEK1 and MEK2 were collected 2.4 Å and 3.2 Å resolution respectively at 100 K on the 17-ID beamline (IMCA) at the Advanced Photon Source Argonne, IL. A wavelength of 1.0 Å was used with crystal to detector distance of 170 mm, with a rotation angle of 0.5 degrees per frame and an exposure time of 10 sec per frame using a MAR CCD for the MEK1 data collection. A wavelength of 1.0 Å was used with crystal to detector distance of 200 mm, with a rotation angle of 0.5 degrees per frame and an exposure time of 10 sec per frame using an ADSC QUANTUM 210 CCD detector was used for the MEK2 data collection.

Example 11: Structural determination of the initial MEK1: ligand: cofactor complex

[0319] Typical crystals of the ternary complex belong to the hexagonal space group, $P6_2$ with unit cell dimensions of approximately a=b=81.4, c=129.2 Å with one molecule per asymmetric unit.

[0320] The initial crystal structure of MEK1 was solved using the SAD method using in-house data from the anomolous signal created by the Iodine atom in the ligand. The data collection statistics are a total of 6699 anomalous pairs out of 25336 measured reflections were found in the resolution range of 36 - 3.4 Å. About 83% of the reflections were measured with a redundancy of 4 and 11% of the reflections were measured with a redundancy of 3, with an overall R_{symm}=0.051.

[0321] All data were processed with HKL2000 and scaled with SCALEPACK (Otwinowski *et al.*, "Processing of x-ray diffraction data collected in oscillation mode," *Methods Enzymol.* 276:307-326 (1997)). All subsequent calculations were done with the CNX package (Molecular Simulations Incorporated). A single position of an iodine atom was found from 3.5 Å anomalous difference Patterson map and later confirmed with the automated Patterson search program. Ten cycles of heavy atom parameters (positional as well as thermal) and phase calculations were performed. An overall figure-of-merit (FOM) was 0.258 for the reflections between 36 and 3.5 Å. Density modification was used to minimize any ambiguity in phase information. A solvent content of 64% was assumed according to a Matthews analyses (Matthews, B.W. *J. Mol. Biol.* 491-497 (1968)). After the density modification procedure, the new phases had FOM=0.858. In order to find a correct enantiomorph similar calculations were done in $P6_5$ space group with flipped positional coordinates of iodine atom. Analyses of the electron density calculated in both space groups confirmed $P6_2$ as a correct one. Phases were extended to 2.38 Å after higher resolution data became available. A 2.38 Å electron density map calculated with these new phases was used for protein model tracing and fitting of the inhibitor and ATP, with the QUNATA-2000 graphical application (Molecular Simulations Incorporated). Atomic models at different stages of completeness were refined with CNX refinement programs (minimize & individual). For the 2.38 Å resolution native data set collected at a wavelength of 1.0 Å at the 17ID line of the APS, a complete sweep of 720 degrees of data was collected. In order to minimize the radiation induced crystal decay only the first 240 out of 720 frames were processed with the HKL2000 and scaled with SCALEPACK. Unit cell dimensions for this crystal were estimated as a=b=81.6, c=129.2 Å. Data included 18590 unique reflections out of 35816 measured in the 36 to 2.38 Å resolution range (about 95 % coverage) with $R_{symm=}$0.044.

Example 12: Refinement of the MEK1: ligand: cofactor structure complexes

[0322] Positional and simulated annealing refinements to the initial structural coordinates were carried out using the

multi-stage maximum likelihood minimization procedure implemented in the program X-PLOR version 98.1 (Accelrys, San Diego, CA.) against data from 25-2.4Å. One round of simulated annealing using the slow-cool procedure (3000 K to 300 K in steps of 25 K) followed by several cycles of standard positional refinement reduced the R_{work} to 0.372 (R_{free} = 0.428). The (2Fo - Fc) and (Fo - Fc) different electron density maps clearly revealed most of the side chains of the model and the binding sites for inhibitor compound (5-bromo-N-(2,3-dihydroxy-propoxy)-3,4-difluoro-2-(2-fluoro-4-iodo-phenylamino)benzamide), ATP and Mg^{2+}. The first round of model rebuilding and positional refinement, followed by individually restrained B-factor refinement reduced the R_{work} to 0.302 (R_{free} = 0.347). Application of bulk solvent correction further reduced the R_{work} to 0.277 (R_{free} = 0.319). The successive rounds of model rebuilding, adding solvent molecules and modeling in the inhibitor and MgATP, followed by positional and restrained individual B refinements produced the current model with R_{work} of 0.223 (R_{free} = 0.276). The current model contains 2159 non-hydrogen protein atoms corresponding to 276 residues of the NH_2-terminally truncated MEK1 in a ternary complex with one ATP molecule, one Mg^{2+} ion, one inhibitor molecule and 80 water molecules.

[0323] The crystal coordinates of the MEK1 peptide (MEK1-C1): Mg-ATP: 5-bromo-N-(2,3-dihydroxy-propoxy)-3,4-difluoro-2-(2-fluoro-4-iodo-phenylamino)benzamide are shown in Table 1.

Example 13: Structural Determination and Refinement of MEK2: ligand: cofactor structure complexes

[0324] Typical crystals of the ternary MEK2 complex belong to the hexagonal space group, $P6_122$ with unit cell dimensions of approximately a=b=161.89, c=122.99 Å with two molecules per asymmetric unit. All data were processed with HKL2000 and scaled with SCALEPACK (Otwinowski *et al.*, "Processing of x-ray diffraction data collected in oscillation mode," *Methods Enzymol.* 276:307-326 (1997)). For the ternary co-complex of MEK2-C2, MgATP and {5-[3,4-Difluoro-2-(2-fluoro-4-iodo-phenylamino)-phenyl]-1,3,4-oxadiazol-2-yl}-(2-morpholin-4-yl-ethyl)-amine, a total of 152,386 measured reflections were identified, with 16,131 unique reflections in the resolution range of 36 - 3.2 Å, with an overall R_{symm}=0.088.

[0325] The structure was solved by molecular replacement using the MEK1: MgATP: inhibitor complex coordinates from Table 1 as a search model using the program Molrep in CCP4 (Collaborative Computational Project, Number 4. 1994. "The CCP4 Suite: Programs for Protein Crystallography". Acta Cryst. D50, 760-763.) A rigid body refinement was performed, followed by one cycle of positional refinement using Refinac in CCP4. A 3.2 Å electron density map was calculated and used for manual fitting of the protein using the program QUNATA-2000 graphical application (Accelrys, San Diego, CA.). Atomic models at different stages of completeness were refined using the CNX refinement programs (minimize & individual).

[0326] Positional and simulated annealing refinements to the initial structural coordinates were carried out using the multi-stage maximum likelihood minimization procedure implemented in the program CNX version 2002 (Accelrys, San Diego, CA.) against data from 25-3.2Å. One round of simulated annealing using the slow-cool procedure (2500 K to 300 K in steps of 25 K) followed by several cycles of standard positional refinement reduced the R_{work} to 0.338 (R_{free} = 0.439). The (2Fo - Fc) and (Fo - Fc) different electron density maps clearly revealed most of the side chains of the model and the binding sites for inhibitor compound {5-[3,4-Difluoro-2-(2-fluoro-4-iodo-phenylamino)-phenyl]-1,3,4-oxadiazol-2-yl}-(2-morpholin-4-yl-ethyl)-amine, ATP and Mg^{2+}. The first round of model rebuilding and positional refinement was followed by modeling in the inhibitor and MgATP. Then positional and group restrained B-factor refinement reduced the R_{work} to 0.29 (R_{free} = 0.37). The crystal coordinates of the MEK2 peptide (MEK2-C2): Mg-ATP: {5-[3,4-Difluoro-2-(2-fluoro-4-iodo-phenylamino)-phenyl]-1,3,4-oxadiazol-2-yl}-(2-morpholin-4-yl-ethyl)-amine are provided in Table 2.

Example 14: Analysis of the crystal structures of the MEK1: ligand: cofactor complexes

[0327] The crystal structure of the ternary complex was obtained in the PDB file format and analyzed using software that performed the functions performed by SYBYL® and REDUCE® software. Initially, the structural data were processed by modifying the atom types of the ligand and cofactor and any waters that were present. The software was then used to titrate the protein by adding all of the hydrogens in the most favorable protonation state, as well as by rotating all the water molecules into orientations that gave the optimal interactions with the protein. After this modification, the protein complexes were ready for binding site characterization and docking simulation. The ligand and cofactor binding sites were characterized using GRIN/GRID® and MOLCAD® contouring. In this procedure, a 4 and 5 Å radius was traced around each atom of the ligand and the cofactor and all the amino acid residues that fell within that radius were identified.

[0328] After analysis of the binding site characterization and the docking studies using the X-ray crystallographic structural data, it was discovered that the MEK1 peptide comprises a ligand-binding pocket that is defined by the structural coordinates of the following amino acid residues within 4 Å of the MEK1 inhibitors located in the ligand-binding site: G77, N78, G79, G80, K97, I99, L115, L118, V127, F129, I141, M143, C207, D208, F209, G210, V211,

S212, L215, I216, M219 of SEQ ID NO: 2. Further, it was discovered that the MEK1 peptide has a ligand-binding pocket that is defined by structural coordinates of the following amino acid residues within 5 Å of the MEK1 inhibitors located in the ligand-binding site: G77, N78, G79, G80, K97, 199, L115, L118, I126, V127, G128, F129, I141, M143, D190, N195, L206, C207, D208, F209, G210, V211, S212, L215, I216, M219, F223 of SEQ ID NO: 2.

[0329] It was also discovered that the MEK1 peptide comprises a cofactor-binding pocket that is defined by the structural coordinates of the following residues within 4 Å of the ATP molecule in the cofactor-binding site: L74, G75, A76, G77, N78, G80, V81, V82, A95, K97, V127, M143, E144, H145, M146, G149, S150, D152, Q153, K192, S194, N195, L197, D208, V224 of SEQ ID NO: 2. Further, it was discovered that the MEK1 peptide comprises a cofactor-binding pocket that is defined by structural coordinates of the following residues within 5 Å of the ATP molecule in the cofactor-binding site: L74, G75, A76, G77, N78, G79, 80, V81, V82, A95, K97, V127, M143, E144, H145, M146, D147, G149, S150, D152, Q153, D190, K192, S194, N195, L197, C207, D208, V224, G225 of SEQ ID NO: 2.

Example 15: Analysis of the crystal structures of the MEK2: ligand: cofactor complexes

[0330] The crystal structure of the ternary complex was obtained in the PDB file format and analyzed using software that performed the functions performed by SYBYL® and REDUCE® software. Initially, the structural data were processed by modifying the atom types of the ligand and cofactor and any waters that were present. The software was then used to titrate the protein by adding all of the hydrogens in the most favorable protonation state, as well as by rotating all the water molecules into orientations that gave the optimal interactions with the protein. After this modification, the protein complexes were ready for binding site characterization and docking simulation. The ligand and cofactor binding sites were characterized using GRIN/GRID® and MOLCAD® contouring. In this procedure, a 4 Å and 5 Å radius was traced around each atom of the ligand and the cofactor and all the amino acid residues that fell within that radius were identified.

[0331] After analysis of the binding site characterization and the docking studies using the X-ray crystallographic structural data, it was discovered that the MEK2 peptide comprises a ligand-binding pocket that is defined by the structural coordinates of the following amino acid residues within 4 Å of the MEK2 inhibitors located in the ligand-binding site: G81, N82, G83, G84, K101, I103, L119, L122, V131, F133, I145, M147, C211, D212, F213, G214, V215, S216, L219, I220, M223 of SEQ ID NO: 4. Further, it was discovered that the MEK2 peptide has a ligand-binding pocket that is defined by structural coordinates of the following amino acid residues within 5 Å of the MEK2 inhibitors located in the ligand-binding site: G81, N82, G83, G84, K101, I103, L119, L122, I130, V131, G132, F133, I145, M147, D194, N199, L210, C211, D212, F213, G214, V215, S216, L219, I220, M223, F227 of SEQ ID NO: 4.

[0332] It was also discovered that the MEK2 peptide comprises a cofactor-binding pocket that is defined by the structural coordinates of the following residues within 4 Å of the ATP molecule in the cofactor-binding site: L78, G79, A80, G81, N82, G84, V85, V86, A99, K101, V131, M147, E148, H149, M150, G153, S154, D156, Q157, K196, S198, N199, L201, D212, V228 of SEQ ID NO: 4. Further, it was discovered that the MEK2 peptide comprises a cofactor-binding pocket that is defined by structural coordinates of the following residues within 5 Å of the ATP molecule in the cofactor-binding site: L78, G79, A80, G81, N82, G83, G84, V85, V86, A99, K101, V131, M147, E148, H149, M150, D151, G153, S154, D156, Q157, D194, K196, S198, N199, L201, C211, D212, V228, G229 of SEQ ID NO: 4.

[0333] After analysis of the binding site characterization and the docking studies using the X-ray crystallographic structural data, it was discovered that certain features of MEK1 and MEK2 are responsible for the high affinity binding of the ligand to the MEK1 or MEK2 ligand binding site. With the inhibitors described above, a binding mode was observed that involves the orientation of the ligand into the hydrophobic prime pocket with a hydrogen bond donor and acceptor interaction with several residues of the activation loop. However, it is expected that continued crystallization of other classes of compounds may reveal novel binding modes that are not currently seen. For example, modeling and docking simulations have revealed alternative binding modes for other more novel classes of compounds. This information can be used, for example, in the evaluation, screening and/or design and modification of a chemical entity that may associate with MEK1 or MEK2 and thus may inhibit MEK1 or MEK2 activity.

[0334] The binding sites according to the invention can serve as a basis for screening a virtual library using various screening techniques known in the art, including, for example, UNITY® (Tripos, Inc.) and any other 3D database screening software. For example, the X-ray crystallographic data found in Table 1 has allowed for the detailed identification of MEK1's three-dimensional structure for the first time. Likewise, the X-ray crystallographic data found in Table 2 has allowed for the detailed identification of MEK2's three-dimensional structure for the first time.

Example 16: Calculation of RMSD's between the MEK1 and MEK2 structures

[0335] The RMS deviations (RMSD's) between the C alpha and/or backbone (N, C, O, and C alpha) atoms of MEK1 and MEK2 structures were calculated herein using the Superimpose command in InsightII (Accelrys). The RMSD's can also be calculated using other modeling programs or scripts. What the Superimpose command does is to perform

a minimum RMS alignment of two molecules on selected sets of atoms from each molecule and output the RMSD value between the selected atoms of the superimposed molecules.

[0336] The RMSD values between several sets of selected C alpha and/or backbone atoms of MEK1 and MEK2 structures have been calculated and listed in Table 8. The RMSD for the C alpha and/or backbone atoms of the overall MEK1 and MEK2 structures was calculated using the following residues: E62-N221, V224-P266, and P307-L381 of MEK1; and E66-N225, V228-P270, and P315-L389 of MEK2. The RMSD for the C alpha and/or backbone atoms of the kinase domain of MEK1 and MEK2 was calculated using the following residues: F68-N221, V224-P266, and P307-I361 of MEK1; and F72-N225, V228-P270, and P315-I369 of MEK2.

[0337] The RMSD for the C alpha and/or backbone atoms of the 4 Å inhibitor binding site residues of MEK1 and MEK2 was calculated using G77, N78, G79, G80, K97, I99, L115, L118, V127, F129, I141, M143, C207, D208, F209, G210, V211, S212, L215, I216 and M219 of SEQ ID NO: 2 (MEK1) and their corresponding residues in MEK2 (Table 2). The RMSD for the C alpha and/or backbone atoms of the 5 Å inhibitor binding site residues of MEK1 and MEK2 was calculated using G77, N78, G79, G80, K97, I99, L115, L118, I126, V127, G128, F129, I141, M143, D190, N195, L206, C207, D208, F209, G210, V211, S212, L215, I216, M219 of SEQ ID NO: 2 (MEK1) and their corresponding residues in MEK2 (Table 2).

[0338] All references cited herein are incorporated by reference in their entirety.

[0339] While the invention has been described in conjunction with examples thereof, it is to be understood that the foregoing description is exemplary and explanatory in nature, and is intended to illustrate the invention and its preferred embodiments. Through routine experimentation, the artisan will recognize apparent modifications and variations that may be made without departing from the spirit of the invention. Thus, the invention is intended to be defined not by the above description, but by the following claims and their equivalents.

[0340] The following Tables are included in the application.

Table 1

Crystal Coordinates of the MEK1: MgATP: 5-bromo-N-(2,3-dihydroxy-propoxy)-3,4-difluoro-2-(2-fluoro-4-iodo-phenylamino)-benzamide Ternary Complex

ATOM	1	CB	GLU	63	1.911	41.776	24.865	1.00	47.12	CDK1
ATOM	2	CG	GLU	63	1.329	43.151	24.968	1.00	43.66	CDK1
ATOM	3	CD	GLU	63	2.206	44.096	25.817	1.00	54.98	CDK1
ATOM	4	OE1	GLU	63	3.094	44.782	25.218	1.00	49.96	CDK1
ATOM	5	OE2	GLU	63	2.016	44.166	27.094	1.00	55.25	CDK1
ATOM	6	C	GLU	63	-0.364	40.840	25.534	1.00	51.68	CDK1
ATOM	7	O	GLU	63	-1.007	41.032	26.560	1.00	60.94	CDK1
ATOM	8	N	GLU	63	1.520	39.342	25.100	1.00	51.25	CDK1
ATOM	9	CA	GLU	63	1.149	40.680	25.628	1.00	49.43	CDK1
ATOM	10	N	LEU	64	-0.961	40.735	24.349	1.00	49.14	CDK1
ATOM	11	CA	LEU	64	-2.422	40.859	24.271	1.00	47.94	CDK1
ATOM	12	CB	LEU	64	-2.840	41.426	22.926	1.00	50.37	CDK1
ATOM	13	CG	LEU	64	-3.452	42.824	22.974	1.00	49.88	CDK1
ATOM	14	CD1	LEU	64	-2.480	43.780	23.629	1.00	43.59	CDK1
ATOM	15	CD2	LEU	64	-3.764	43.289	21.575	1.00	43.10	CDK1
ATOM	16	C	LEU	64	-3.133	39.520	24.516	1.00	53.50	CDK1
ATOM	17	O	LEU	64	-2.899	38.550	23.797	1.00	56.21	CDK1
ATOM	18	N	LYS	65	-3.989	39.481	25.546	1.00	57.95	CDK1
ATOM	19	CA	LYS	65	-4.750	38.278	25.952	1.00	56.48	CDK1
ATOM	20	CB	LYS	65	-4.444	37.916	27.414	1.00	58.05	CDK1
ATOM	21	CG	LYS	65	-3.065	37.326	27.659	1.00	62.60	CDK1
ATOM	22	CD	LYS	65	-3.003	36.592	29.002	1.00	62.37	CDK1
ATOM	23	CE	LYS	65	-3.085	37.556	30.173	1.00	61.71	CDK1
ATOM	24	NZ	LYS	65	-4.391	37.461	30.884	1.00	51.87	CDK1
ATOM	25	C	LYS	65	-6.269	38.455	25.821	1.00	55.10	CDK1
ATOM	26	O	LYS	65	-6.778	39.577	25.841	1.00	56.94	CDK1
ATOM	27	N	ASP	66	-6.998	37.348	25.720	1.00	51.16	CDK1
ATOM	28	CA	ASP	66	-8.451	37.421	25.585	1.00	50.31	CDK1
ATOM	29	CB	ASP	66	-9.027	36.029	25.312	1.00	48.53	CDK1
ATOM	30	CG	ASP	66	-10.550	36.031	25.221	1.00	49.64	CDK1
ATOM	31	OD1	ASP	66	-11.142	36.969	24.642	1.00	51.91	CDK1
ATOM	32	OD2	ASP	66	-11.169	35.080	25.730	1.00	60.30	CDK1
ATOM	33	C	ASP	66	-9.133	38.022	26.820	1.00	53.61	CDK1

ATOM	34	O	ASP	66	-10.058	38.834	26.697	1.00	49.78	CDK1
ATOM	35	N	ASP	67	-8.663	37.632	28.004	1.00	56.17	CDK1
ATOM	36	CA	ASP	67	-9.236	38.109	29.267	1.00	60.12	CDK1
ATOM	37	CB	ASP	67	-8.711	37.288	30.454	1.00	64.33	CDK1
ATOM	38	CG	ASP	67	-7.494	36.449	30.105	1.00	78.36	CDK1
ATOM	39	OD1	ASP	67	-7.421	35.910	28.974	1.00	84.85	CDK1
ATOM	40	OD2	ASP	67	-6.604	36.322	30.977	1.00	84.15	CDK1
ATOM	41	C	ASP	67	-9.031	39.594	29.557	1.00	56.52	CDK1
ATOM	42	O	ASP	67	-9.896	40.231	30.158	1.00	56.00	CDK1
ATOM	43	N	ASP	68	-7.904	40.149	29.127	1.00	49.31	CDK1
ATOM	44	CA	ASP	68	-7.625	41.557	29.363	1.00	43.05	CDK1
ATOM	45	CB	ASP	68	-6.148	41.823	29.100	1.00	47.50	CDK1
ATOM	46	CG	ASP	68	-5.248	40.983	29.989	1.00	52.01	CDK1
ATOM	47	OD1	ASP	68	-4.007	41.147	29.953	1.00	46.97	CDK1
ATOM	48	OD2	ASP	68	-5.797	40.147	30.734	1.00	56.12	CDK1
ATOM	49	C	ASP	68	-8.486	42.549	28.577	1.00	43.93	CDK1
ATOM	50	O	ASP	68	-8.183	43.742	28.573	1.00	45.17	CDK1
ATOM	51	N	PHE	69	-9.562	42.067	27.942	1.00	41.39	CDK1
ATOM	52	CA	PHE	69	-10.460	42.918	27.139	1.00	40.09	CDK1
ATOM	53	CB	PHE	69	-10.586	42.395	25.690	1.00	38.16	CDK1
ATOM	54	CG	PHE	69	-9.408	42.706	24.828	1.00	33.20	CDK1
ATOM	55	CD1	PHE	69	-9.234	43.977	24.321	1.00	30.42	CDK1
ATOM	56	CD2	PHE	69	-8.425	41.750	24.606	1.00	31.00	CDK1
ATOM	57	CE1	PHE	69	-8.089	44.299	23.619	1.00	34.47	CDK1
ATOM	58	CE2	PHE	69	-7.270	42.062	23.901	1.00	30.56	CDK1
ATOM	59	CZ	PHE	69	-7.095	43.338	23.408	1.00	25.48	CDK1
ATOM	60	C	PHE	69	-11.861	42.941	27.701	1.00	40.30	CDK1
ATOM	61	O	PHE	69	-12.258	42.014	28.376	1.00	40.70	CDK1
ATOM	62	N	GLU	70	-12.623	43.979	27.373	1.00	43.63	CDK1
ATOM	63	CA	GLU	70	-14.011	44.089	27.816	1.00	48.94	CDK1
ATOM	64	CB	GLU	70	-14.103	44.936	29.101	1.00	56.95	CDK1
ATOM	65	CG	GLU	70	-15.501	45.449	29.450	1.00	61.99	CDK1
ATOM	66	CD	GLU	70	-15.596	46.979	29.421	1.00	73.96	CDK1
ATOM	67	OE1	GLU	70	-14.553	47.654	29.589	1.00	76.19	CDK1
ATOM	68	OE2	GLU	70	-16.717	47.511	29.230	1.00	77.39	CDK1
ATOM	69	C	GLU	70	-14.817	44.736	26.688	1.00	49.67	CDK1
ATOM	70	O	GLU	70	-14.461	45.804	26.179	1.00	47.32	CDK1
ATOM	71	N	LYS	71	-15.904	44.087	26.296	1.00	48.53	CDK1
ATOM	72	CA	LYS	71	-16.730	44.603	25.214	1.00	51.94	CDK1
ATOM	73	CB	LYS	71	-17.830	43.590	24.866	1.00	53.44	CDK1
ATOM	74	CG	LYS	71	-17.931	43.211	23.398	1.00	55.21	CDK1
ATOM	75	CD	LYS	71	-17.570	41.734	23.195	1.00	62.97	CDK1
ATOM	76	CE	LYS	71	-18.789	40.879	22.829	1.00	61.29	CDK1

ATOM	77	NZ	LYS	71	-20.072	41.651	22.889	1.00 62.20	CDK1
ATOM	78	C	LYS	71	-17.364	45.937	25.573	1.00 52.10	CDK1
ATOM	79	O	LYS	71	-18.006	46.055	26.606	1.00 57.97	CDK1
ATOM	80	N	ILE	72	-17.185	46.937	24.717	1.00 51.76	CDK1
ATOM	81	CA	ILE	72	-17.778	48.253	24.930	1.00 50.77	CDK1
ATOM	82	CB	ILE	72	-16.820	49.385	24.520	1.00 48.80	CDK1
ATOM	83	CG2	ILE	72	-17.584	50.679	24.368	1.00 41.25	CDK1
ATOM	84	CG1	ILE	72	-15.715	49.545	25.563	1.00 49.54	CDK1
ATOM	85	CD1	ILE	72	-14.608	50.498	25.130	1.00 52.47	CDK1
ATOM	86	C	ILE	72	-19.029	48.346	24.058	1.00 58.25	CDK1
ATOM	87	O	ILE	72	-20.152	48.307	24.565	1.00 59.88	CDK1
ATOM	88	N	SER	73	-18.822	48.464	22.745	1.00 60.54	CDK1
ATOM	89	CA	SER	73	-19.922	48.546	21.788	1.00 62.18	CDK1
ATOM	90	CB	SER	73	-20.277	50.004	21.526	1.00 62.22	CDK1
ATOM	91	OG	SER	73	-19.595	50.476	20.385	1.00 72.58	CDK1
ATOM	92	C	SER	73	-19.609	47.842	20.460	1.00 61.03	CDK1
ATOM	93	O	SER	73	-18.469	47.463	20.188	1.00 65.74	CDK1
ATOM	94	N	GLU	74	-20.636	47.667	19.640	1.00 60.49	CDK1
ATOM	95	CA	GLU	74	-20.503	46.997	18.342	1.00 61.43	CDK1
ATOM	96	CB	GLU	74	-21.804	46.253	18.032	1.00 61.77	CDK1
ATOM	97	CG	GLU	74	-22.028	45.950	16.570	1.00 74.67	CDK1
ATOM	98	CD	GLU	74	-21.712	44.508	16.232	1.00 82.79	CDK1
ATOM	99	OE1	GLU	74	-22.506	43.888	15.488	1.00 85.38	CDK1
ATOM	100	OE2	GLU	74	-20.670	43.998	16.711	1.00 86.15	CDK1
ATOM	101	C	GLU	74	-20.182	47.989	17.214	1.00 57.99	CDK1
ATOM	102	O	GLU	74	-20.972	48.890	16.942	1.00 57.45	CDK1
ATOM	103	N	LEU	75	-19.037	47.812	16.551	1.00 54.73	CDK1
ATOM	104	CA	LEU	75	-18.628	48.718	15.471	1.00 54.78	CDK1
ATOM	105	CB	LEU	75	-17.102	48.739	15.359	1.00 51.93	CDK1
ATOM	106	CG	LEU	75	-16.384	49.546	16.440	1.00 41.57	CDK1
ATOM	107	CD1	LEU	75	-14.897	49.267	16.417	1.00 35.33	CDK1
ATOM	108	CD2	LEU	75	-16.674	51.021	16.215	1.00 43.91	CDK1
ATOM	109	C	LEU	75	-19.233	48.406	14.096	1.00 55.61	CDK1
ATOM	110	O	LEU	75	-19.424	49.301	13.284	1.00 54.15	CDK1
ATOM	111	N	GLY	76	-19.534	47.136	13.848	1.00 55.37	CDK1
ATOM	112	CA	GLY	76	-20.113	46.735	12.586	1.00 53.17	CDK1
ATOM	113	C	GLY	76	-19.905	45.247	12.405	1.00 60.26	CDK1
ATOM	114	O	GLY	76	-19.228	44.608	13.224	1.00 56.56	CDK1
ATOM	115	N	ALA	77	-20.499	44.690	11.349	1.00 64.98	CDK1
ATOM	116	CA	ALA	77	-20.367	43.266	11.038	1.00 67.86	CDK1
ATOM	117	CB	ALA	77	-21.596	42.501	11.492	1.00 67.58	CDK1
ATOM	118	C	ALA	77	-20.204	43.118	9.540	1.00 68.86	CDK1
ATOM	119	O	ALA	77	-20.741	43.921	8.775	1.00 68.97	CDK1

ATOM	120	N	GLY	78	-19.464	42.096	9.125	1.00	68.72	CDK1
ATOM	121	CA	GLY	78	-19.260	41.875	7.709	1.00	70.24	CDK1
ATOM	122	C	GLY	78	-19.598	40.458	7.310	1.00	73.13	CDK1
ATOM	123	O	GLY	78	-20.221	39.721	8.074	1.00	71.82	CDK1
ATOM	124	N	ASN	79	-19.199	40.084	6.099	1.00	77.45	CDK1
ATOM	125	CA	ASN	79	-19.428	38.736	5.587	1.00	81.51	CDK1
ATOM	126	CB	ASN	79	-19.041	38.645	4.108	1.00	86.42	CDK1
ATOM	127	CG	ASN	79	-20.248	38.580	3.193	1.00	92.12	CDK1
ATOM	128	OD1	ASN	79	-20.794	39.611	2.786	1.00	95.79	CDK1
ATOM	129	ND2	ASN	79	-20.673	37.363	2.860	1.00	94.64	CDK1
ATOM	130	C	ASN	79	-18.533	37.834	6.420	1.00	80.68	CDK1
ATOM	131	O	ASN	79	-17.631	37.159	5.912	1.00	78.09	CDK1
ATOM	132	N	GLY	80	-18.799	37.852	7.718	1.00	79.54	CDK1
ATOM	133	CA	GLY	80	-18.031	37.075	8.660	1.00	82.19	CDK1
ATOM	134	C	GLY	80	-17.778	37.931	9.882	1.00	82.11	CDK1
ATOM	135	O	GLY	80	-18.707	38.500	10.471	1.00	83.24	CDK1
ATOM	136	N	GLY	81	-16.509	38.035	10.250	1.00	81.24	CDK1
ATOM	137	CA	GLY	81	-16.127	38.815	11.409	1.00	78.16	CDK1
ATOM	138	C	GLY	81	-17.010	39.984	11.804	1.00	74.13	CDK1
ATOM	139	O	GLY	81	-17.522	40.736	10.972	1.00	71.77	CDK1
ATOM	140	N	VAL	82	-17.227	40.100	13.106	1.00	73.17	CDK1
ATOM	141	CA	VAL	82	-17.983	41.214	13.652	1.00	66.83	CDK1
ATOM	142	CB	VAL	82	-19.064	40.775	14.643	1.00	65.38	CDK1
ATOM	143	CG1	VAL	82	-18.420	40.170	15.887	1.00	64.61	CDK1
ATOM	144	CG2	VAL	82	-19.930	41.966	14.997	1.00	56.65	CDK1
ATOM	145	C	VAL	82	-16.862	41.926	14.389	1.00	61.57	CDK1
ATOM	146	O	VAL	82	-15.899	41.287	14.830	1.00	58.85	CDK1
ATOM	147	N	VAL	83	-16.956	43.238	14.501	1.00	55.91	CDK1
ATOM	148	CA	VAL	83	-15.887	43.961	15.151	1.00	53.12	CDK1
ATOM	149	CB	VAL	83	-15.064	44.764	14.092	1.00	56.58	CDK1
ATOM	150	CG1	VAL	83	-16.003	45.405	13.083	1.00	60.32	CDK1
ATOM	151	CG2	VAL	83	-14.174	45.804	14.760	1.00	44.19	CDK1
ATOM	152	C	VAL	83	-16.429	44.849	16.251	1.00	50.23	CDK1
ATOM	153	O	VAL	83	-17.302	45.703	16.043	1.00	44.02	CDK1
ATOM	154	N	PHE	84	-15.899	44.619	17.442	1.00	50.96	CDK1
ATOM	155	CA	PHE	84	-16.322	45.355	18.618	1.00	47.93	CDK1
ATOM	156	CB	PHE	84	-16.435	44.409	19.815	1.00	48.47	CDK1
ATOM	157	CG	PHE	84	-17.317	43.207	19.582	1.00	50.89	CDK1
ATOM	158	CD1	PHE	84	-16.759	41.942	19.422	1.00	50.80	CDK1
ATOM	159	CD2	PHE	84	-18.707	43.327	19.614	1.00	52.86	CDK1
ATOM	160	CE1	PHE	84	-17.574	40.809	19.306	1.00	52.24	CDK1
ATOM	161	CE2	PHE	84	-19.533	42.202	19.502	1.00	48.57	CDK1
ATOM	162	CZ	PHE	84	-18.965	40.943	19.350	1.00	51.67	CDK1

ATOM	163	C	PHE	84	-15.380	46.473	19.004	1.00 46.06	CDK1
ATOM	164	O	PHE	84	-14.150	46.342	18.897	1.00 41.74	CDK1
ATOM	165	N	LYS	85	-15.967	47.582	19.444	1.00 44.27	CDK1
ATOM	166	CA	LYS	85	-15.169	48.687	19.953	1.00 45.57	CDK1
ATOM	167	CB	LYS	85	-16.000	49.955	20.051	1.00 47.54	CDK1
ATOM	168	CG	LYS	85	-15.527	50.888	21.138	1.00 51.54	CDK1
ATOM	169	CD	LYS	85	-15.515	52.311	20.649	1.00 53.90	CDK1
ATOM	170	CE	LYS	85	-16.382	53.194	21.523	1.00 50.73	CDK1
ATOM	171	NZ	LYS	85	-15.664	54.466	21.841	1.00 57.37	CDK1
ATOM	172	C	LYS	85	-14.901	48.160	21.358	1.00 48.89	CDK1
ATOM	173	O	LYS	85	-15.844	47.863	22.082	1.00 48.31	CDK1
ATOM	174	N	VAL	86	-13.642	48.013	21.750	1.00 48.98	CDK1
ATOM	175	CA	VAL	86	-13.369	47.484	23.072	1.00 44.37	CDK1
ATOM	176	CB	VAL	86	-12.948	45.993	23.022	1.00 42.84	CDK1
ATOM	177	CG1	VAL	86	-13.931	45.197	22.193	1.00 44.53	CDK1
ATOM	178	CG2	VAL	86	-11.532	45.868	22.474	1.00 45.66	CDK1
ATOM	179	C	VAL	86	-12.307	48.214	23.862	1.00 47.62	CDK1
ATOM	180	O	VAL	86	-11.640	49.131	23.368	1.00 46.67	CDK1
ATOM	181	N	SER	87	-12.162	47.781	25.113	1.00 47.01	CDK1
ATOM	182	CA	SER	87	-11.175	48.349	26.012	1.00 42.71	CDK1
ATOM	183	CB	SER	87	-11.841	48.900	27.276	1.00 47.77	CDK1
ATOM	184	OG	SER	87	-11.176	50.070	27.727	1.00 50.76	CDK1
ATOM	185	C	SER	87	-10.168	47.291	26.403	1.00 33.62	CDK1
ATOM	186	O	SER	87	-10.531	46.174	26.766	1.00 36.85	CDK1
ATOM	187	N	HIS	88	-8.894	47.626	26.290	1.00 26.31	CDK1
ATOM	188	CA	HIS	88	-7.870	46.689	26.701	1.00 32.04	CDK1
ATOM	189	CB	HIS	88	-6.637	46.857	25.827	1.00 23.47	CDK1
ATOM	190	CG	HIS	88	-5.485	46.014	26.260	1.00 21.27	CDK1
ATOM	191	CD2	HIS	88	-5.379	44.677	26.453	1.00 21.42	CDK1
ATOM	192	ND1	HIS	88	-4.244	46.545	26.549	1.00 28.91	CDK1
ATOM	193	CE1	HIS	88	-3.420	45.569	26.900	1.00 28.99	CDK1
ATOM	194	NE2	HIS	88	-4.083	44.426	26.851	1.00 24.28	CDK1
ATOM	195	C	HIS	88	-7.591	47.108	28.167	1.00 35.46	CDK1
ATOM	196	O	HIS	88	-6.864	48.067	28.427	1.00 29.93	CDK1
ATOM	197	N	LYS	89	-8.190	46.390	29.113	1.00 36.24	CDK1
ATOM	198	CA	LYS	89	-8.066	46.721	30.536	1.00 40.58	CDK1
ATOM	199	CB	LYS	89	-8.687	45.617	31.387	1.00 44.05	CDK1
ATOM	200	CG	LYS	89	-10.211	45.664	31.377	1.00 51.48	CDK1
ATOM	201	CD	LYS	89	-10.812	44.497	32.149	1.00 52.19	CDK1
ATOM	202	CE	LYS	89	-10.426	43.160	31.544	1.00 52.76	CDK1
ATOM	203	NZ	LYS	89	-11.391	42.103	31.962	1.00 54.49	CDK1
ATOM	204	C	LYS	89	-6.682	47.057	31.064	1.00 35.19	CDK1
ATOM	205	O	LYS	89	-6.498	48.069	31.707	1.00 36.45	CDK1

ATOM	206	N	PRO	90	-5.688	46.225	30.787	1.00	33.18	CDK1
ATOM	207	CD	PRO	90	-5.685	44.957	30.043	1.00	31.41	CDK1
ATOM	208	CA	PRO	90	-4.368	46.571	31.309	1.00	30.45	CDK1
ATOM	209	CB	PRO	90	-3.487	45.400	30.880	1.00	28.71	CDK1
ATOM	210	CG	PRO	90	-4.463	44.270	30.574	1.00	23.30	CDK1
ATOM	211	C	PRO	90	-3.783	47.904	30.863	1.00	39.35	CDK1
ATOM	212	O	PRO	90	-2.958	48.494	31.575	1.00	47.08	CDK1
ATOM	213	N	SER	91	-4.200	48.405	29.704	1.00	39.40	CDK1
ATOM	214	CA	SER	91	-3.616	49.650	29.222	1.00	33.27	CDK1
ATOM	215	CB	SER	91	-3.004	49.428	27.830	1.00	34.00	CDK1
ATOM	216	OG	SER	91	-4.007	49.533	26.820	1.00	37.38	CDK1
ATOM	217	C	SER	91	-4.563	50.832	29.178	1.00	29.42	CDK1
ATOM	218	O	SER	91	-4.128	51.984	29.105	1.00	31.11	CDK1
ATOM	219	N	GLY	92	-5.855	50.555	29.212	1.00	31.04	CDK1
ATOM	220	CA	GLY	92	-6.837	51.627	29.144	1.00	33.29	CDK1
ATOM	221	C	GLY	92	-7.103	52.092	27.713	1.00	37.82	CDK1
ATOM	222	O	GLY	92	-7.943	52.963	27.473	1.00	39.74	CDK1
ATOM	223	N	LEU	93	-6.383	51.517	26.756	1.00	40.09	CDK1
ATOM	224	CA	LEU	93	-6.557	51.886	25.349	1.00	39.55	CDK1
ATOM	225	CB	LEU	93	-5.416	51.335	24.497	1.00	39.71	CDK1
ATOM	226	CG	LEU	93	-4.104	52.104	24.448	1.00	44.79	CDK1
ATOM	227	CD1	LEU	93	-3.092	51.348	23.574	1.00	41.83	CDK1
ATOM	228	CD2	LEU	93	-4.377	53.503	23.917	1.00	47.22	CDK1
ATOM	229	C	LEU	93	-7.846	51.339	24.783	1.00	33.39	CDK1
ATOM	230	O	LEU	93	-8.157	50.168	24.966	1.00	38.01	CDK1
ATOM	231	N	VAL	94	-8.610	52.189	24.113	1.00	38.49	CDK1
ATOM	232	CA	VAL	94	-9.825	51.725	23.472	1.00	42.84	CDK1
ATOM	233	CB	VAL	94	-10.759	52.884	23.183	1.00	48.07	CDK1
ATOM	234	CG1	VAL	94	-11.827	52.453	22.201	1.00	49.00	CDK1
ATOM	235	CG2	VAL	94	-11.390	53.349	24.474	1.00	46.68	CDK1
ATOM	236	C	VAL	94	-9.301	51.134	22.154	1.00	42.55	CDK1
ATOM	237	O	VAL	94	-8.453	51.731	21.513	1.00	37.15	CDK1
ATOM	238	N	MET	95	-9.762	49.949	21.776	1.00	43.79	CDK1
ATOM	239	CA	MET	95	-9.294	49.316	20.544	1.00	41.17	CDK1
ATOM	240	CB	MET	95	-8.346	48.144	20.882	1.00	36.23	CDK1
ATOM	241	CG	MET	95	-7.031	48.579	21.544	1.00	35.68	CDK1
ATOM	242	SD	MET	95	-5.769	47.282	21.958	1.00	43.36	CDK1
ATOM	243	CE	MET	95	-6.647	45.910	21.684	1.00	37.22	CDK1
ATOM	244	C	MET	95	-10.475	48.808	19.715	1.00	43.77	CDK1
ATOM	245	O	MET	95	-11.632	48.923	20.126	1.00	45.55	CDK1
ATOM	246	N	ALA	96	-10.186	48.288	18.523	1.00	44.44	CDK1
ATOM	247	CA	ALA	96	-11.227	47.713	17.672	1.00	38.61	CDK1
ATOM	248	CB	ALA	96	-11.218	48.330	16.292	1.00	40.19	CDK1

ATOM	249	C	ALA	96	-10.778	46.275	17.623	1.00 34.38	CDK1
ATOM	250	O	ALA	96	-9.607	45.994	17.372	1.00 33.58	CDK1
ATOM	251	N	ARG	97	-11.697	45.369	17.911	1.00 34.08	CDK1
ATOM	252	CA	ARG	97	-11.359	43.958	17.950	1.00 38.52	CDK1
ATOM	253	CB	ARG	97	-11.665	43.375	19.331	1.00 33.96	CDK1
ATOM	254	CG	ARG	97	-10.924	42.086	19.627	1.00 36.60	CDK1
ATOM	255	CD	ARG	97	-11.670	41.212	20.626	1.00 32.78	CDK1
ATOM	256	NE	ARG	97	-10.915	39.987	20.891	1.00 35.53	CDK1
ATOM	257	CZ	ARG	97	-11.155	39.155	21.900	1.00 43.85	CDK1
ATOM	258	NH1	ARG	97	-12.137	39.406	22.754	1.00 42.34	CDK1
ATOM	259	NH2	ARG	97	-10.405	38.073	22.059	1.00 42.46	CDK1
ATOM	260	C	ARG	97	-12.143	43.197	16.904	1.00 40.90	CDK1
ATOM	261	O	ARG	97	-13.378	43.191	16.933	1.00 36.53	CDK1
ATOM	262	N	LYS	98	-11.413	42.560	15.989	1.00 36.10	CDK1
ATOM	263	CA	LYS	98	-12.036	41.788	14.926	1.00 36.12	CDK1
ATOM	264	CB	LYS	98	-11.364	42.071	13.579	1.00 37.72	CDK1
ATOM	265	CG	LYS	98	-12.230	41.670	12.395	1.00 42.54	CDK1
ATOM	266	CD	LYS	98	-11.411	41.124	11.248	1.00 44.17	CDK1
ATOM	267	CE	LYS	98	-11.118	42.226	10.226	1.00 44.61	CDK1
ATOM	268	NZ	LYS	98	-12.304	42.541	9.393	1.00 40.71	CDK1
ATOM	269	C	LYS	98	-11.930	40.308	15.235	1.00 33.57	CDK1
ATOM	270	O	LYS	98	-10.840	39.797	15.528	1.00 29.10	CDK1
ATOM	271	N	LEU	99	-13.072	39.627	15.180	1.00 33.62	CDK1
ATOM	272	CA	LEU	99	-13.115	38.189	15.439	1.00 41.28	CDK1
ATOM	273	CB	LEU	99	-14.215	37.850	16.465	1.00 41.70	CDK1
ATOM	274	CG	LEU	99	-14.113	38.226	17.954	1.00 43.80	CDK1
ATOM	275	CD1	LEU	99	-12.674	38.170	18.450	1.00 40.92	CDK1
ATOM	276	CD2	LEU	99	-14.694	39.611	18.134	1.00 42.47	CDK1
ATOM	277	C	LEU	99	-13.415	37.437	14.136	1.00 43.56	CDK1
ATOM	278	O	LEU	99	-14.455	37.658	13.514	1.00 39.81	CDK1
ATOM	279	N	ILE	100	-12.509	36.554	13.731	1.00 44.07	CDK1
ATOM	280	CA	ILE	100	-12.714	35.766	12.520	1.00 45.79	CDK1
ATOM	281	CB	ILE	100	-11.501	35.862	11.546	1.00 44.29	CDK1
ATOM	282	CG2	ILE	100	-11.695	34.931	10.363	1.00 35.49	CDK1
ATOM	283	CG1	ILE	100	-11.351	37.282	11.024	1.00 38.35	CDK1
ATOM	284	CD1	ILE	100	-9.991	37.549	10.447	1.00 43.96	CDK1
ATOM	285	C	ILE	100	-12.833	34.335	12.986	1.00 46.58	CDK1
ATOM	286	O	ILE	100	-11.868	33.791	13.505	1.00 46.37	CDK1
ATOM	287	N	HIS	101	-13.999	33.725	12.802	1.00 51.41	CDK1
ATOM	288	CA	HIS	101	-14.182	32.353	13.244	1.00 61.90	CDK1
ATOM	289	CB	HIS	101	-15.517	31.788	12.776	1.00 71.49	CDK1
ATOM	290	CG	HIS	101	-15.936	30.545	13.509	1.00 81.14	CDK1
ATOM	291	CD2	HIS	101	-15.750	29.232	13.223	1.00 84.78	CDK1

ATOM	292	ND1	HIS	101	-16.649	30.579	14.690	1.00	84.74	CDK1
ATOM	293	CE1	HIS	101	-16.883	29.343	15.097	1.00	86.15	CDK1
ATOM	294	NE2	HIS	101	-16.348	28.507	14.225	1.00	84.95	CDK1
ATOM	295	C	HIS	101	-13.059	31.464	12.751	1.00	67.25	CDK1
ATOM	296	O	HIS	101	-11.965	31.488	13.312	1.00	74.70	CDK1
ATOM	297	N	LEU	102	-13.327	30.672	11.719	1.00	67.82	CDK1
ATOM	298	CA	LEU	102	-12.320	29.772	11.154	1.00	73.45	CDK1
ATOM	299	CB	LEU	102	-10.943	30.451	11.128	1.00	69.76	CDK1
ATOM	300	CG	LEU	102	-10.498	31.193	9.867	1.00	69.16	CDK1
ATOM	301	CD1	LEU	102	-11.711	31.672	9.081	1.00	66.05	CDK1
ATOM	302	CD2	LEU	102	-9.618	32.362	10.267	1.00	68.00	CDK1
ATOM	303	C	LEU	102	-12.178	28.421	11.862	1.00	77.61	CDK1
ATOM	304	O	LEU	102	-11.366	28.278	12.778	1.00	78.63	CDK1
ATOM	305	N	GLU	103	-12.961	27.432	11.437	1.00	82.39	CDK1
ATOM	306	CA	GLU	103	-12.869	26.095	12.016	1.00	85.59	CDK1
ATOM	307	CB	GLU	103	-14.034	25.225	11.554	1.00	89.41	CDK1
ATOM	308	CG	GLU	103	-15.318	25.413	12.329	1.00	92.70	CDK1
ATOM	309	CD	GLU	103	-16.516	24.848	11.584	1.00	97.14	CDK1
ATOM	310	OE1	GLU	103	-17.662	25.160	11.973	1.00	99.14	CDK1
ATOM	311	OE2	GLU	103	-16.310	24.090	10.606	1.00	98.54	CDK1
ATOM	312	C	GLU	103	-11.572	25.530	11.456	1.00	86.27	CDK1
ATOM	313	O	GLU	103	-11.570	24.861	10.419	1.00	84.90	CDK1
ATOM	314	N	ILE	104	-10.470	25.807	12.142	1.00	86.88	CDK1
ATOM	315	CA	ILE	104	-9.169	25.357	11.681	1.00	86.24	CDK1
ATOM	316	CB	ILE	104	-8.424	26.549	11.013	1.00	87.91	CDK1
ATOM	317	CG2	ILE	104	-7.167	26.917	11.792	1.00	87.65	CDK1
ATOM	318	CG1	ILE	104	-8.117	26.201	9.554	1.00	89.75	CDK1
ATOM	319	CD1	ILE	104	-9.357	25.980	8.691	1.00	89.86	CDK1
ATOM	320	C	ILE	104	-8.311	24.715	12.775	1.00	85.28	CDK1
ATOM	321	O	ILE	104	-8.389	25.088	13.947	1.00	84.21	CDK1
ATOM	322	N	ALA	105	-7.499	23.741	12.373	1.00	84.76	CDK1
ATOM	323	CA	ALA	105	-6.623	23.026	13.291	1.00	83.74	CDK1
ATOM	324	CB	ALA	105	-6.049	21.789	12.618	1.00	82.13	CDK1
ATOM	325	C	ALA	105	-5.497	23.920	13.769	1.00	85.19	CDK1
ATOM	326	O	ALA	105	-4.932	24.699	13.002	1.00	83.35	CDK1
ATOM	327	N	PRO	106	-5.154	23.813	15.055	1.00	88.28	CDK1
ATOM	328	CD	PRO	106	-5.790	22.910	16.036	1.00	88.80	CDK1
ATOM	329	CA	PRO	106	-4.084	24.617	15.655	1.00	88.28	CDK1
ATOM	330	CB	PRO	106	-3.792	23.891	16.966	1.00	89.78	CDK1
ATOM	331	CG	PRO	106	-5.121	23.279	17.338	1.00	89.44	CDK1
ATOM	332	C	PRO	106	-2.837	24.791	14.786	1.00	85.45	CDK1
ATOM	333	O	PRO	106	-2.149	25.807	14.879	1.00	85.86	CDK1
ATOM	334	N	ALA	107	-2.556	23.810	13.936	1.00	81.97	CDK1

ATOM	335	CA	ALA	107	-1.380	23.875	13.075	1.00	81.68	CDK1
ATOM	336	CB	ALA	107	-1.303	22.628	12.199	1.00	83.93	CDK1
ATOM	337	C	ALA	107	-1.384	25.125	12.203	1.00	81.35	CDK1
ATOM	338	O	ALA	107	-0.430	25.906	12.207	1.00	81.76	CDK1
ATOM	339	N	ILE	108	-2.463	25.312	11.454	1.00	78.50	CDK1
ATOM	340	CA	ILE	108	-2.577	26.459	10.573	1.00	75.53	CDK1
ATOM	341	CB	ILE	108	-3.633	26.205	9.460	1.00	75.16	CDK1
ATOM	342	CG2	ILE	108	-4.219	24.814	9.600	1.00	72.14	CDK1
ATOM	343	CG1	ILE	108	-4.746	27.248	9.519	1.00	76.59	CDK1
ATOM	344	CD1	ILE	108	-5.515	27.365	8.231	1.00	77.95	CDK1
ATOM	345	C	ILE	108	-2.936	27.703	11.365	1.00	73.53	CDK1
ATOM	346	O	ILE	108	-2.375	28.780	11.145	1.00	70.18	CDK1
ATOM	347	N	ARG	109	-3.880	27.551	12.284	1.00	72.26	CDK1
ATOM	348	CA	ARG	109	-4.302	28.666	13.112	1.00	74.10	CDK1
ATOM	349	CB	ARG	109	-5.252	28.156	14.213	1.00	76.96	CDK1
ATOM	350	CG	ARG	109	-5.118	28.783	15.597	1.00	79.46	CDK1
ATOM	351	CD	ARG	109	-4.517	27.788	16.584	1.00	85.84	CDK1
ATOM	352	NE	ARG	109	-5.505	27.075	17.401	1.00	93.07	CDK1
ATOM	353	CZ	ARG	109	-6.448	26.258	16.927	1.00	95.63	CDK1
ATOM	354	NH1	ARG	109	-6.554	26.037	15.624	1.00	96.95	CDK1
ATOM	355	NH2	ARG	109	-7.276	25.636	17.759	1.00	92.83	CDK1
ATOM	356	C	ARG	109	-3.037	29.307	13.685	1.00	73.72	CDK1
ATOM	357	O	ARG	109	-2.964	30.517	13.894	1.00	73.53	CDK1
ATOM	358	N	ASN	110	-2.016	28.494	13.898	1.00	73.68	CDK1
ATOM	359	CA	ASN	110	-0.779	29.023	14.437	1.00	75.47	CDK1
ATOM	360	CB	ASN	110	-0.009	27.911	15.150	1.00	80.16	CDK1
ATOM	361	CG	ASN	110	-0.404	27.791	16.614	1.00	84.31	CDK1
ATOM	362	OD1	ASN	110	0.114	28.516	17.465	1.00	86.63	CDK1
ATOM	363	ND2	ASN	110	-1.334	26.887	16.911	1.00	84.03	CDK1
ATOM	364	C	ASN	110	0.055	29.663	13.336	1.00	71.95	CDK1
ATOM	365	O	ASN	110	0.922	30.498	13.599	1.00	71.80	CDK1
ATOM	366	N	GLN	111	-0.223	29.270	12.099	1.00	66.89	CDK1
ATOM	367	CA	GLN	111	0.471	29.824	10.943	1.00	61.97	CDK1
ATOM	368	CB	GLN	111	0.151	29.000	9.699	1.00	65.42	CDK1
ATOM	369	CG	GLN	111	1.341	28.299	9.101	1.00	69.69	CDK1
ATOM	370	CD	GLN	111	1.901	29.048	7.932	1.00	72.85	CDK1
ATOM	371	OE1	GLN	111	2.916	29.743	8.051	1.00	77.37	CDK1
ATOM	372	NE2	GLN	111	1.245	28.920	6.784	1.00	69.82	CDK1
ATOM	373	C	GLN	111	-0.059	31.236	10.748	1.00	56.49	CDK1
ATOM	374	O	GLN	111	0.698	32.199	10.593	1.00	52.79	CDK1
ATOM	375	N	ILE	112	-1.382	31.333	10.760	1.00	51.92	CDK1
ATOM	376	CA	ILE	112	-2.071	32.598	10.586	1.00	49.17	CDK1
ATOM	377	CB	ILE	112	-3.586	32.385	10.706	1.00	45.37	CDK1

ATOM	378	CG2	ILE	112	-4.320	33.725	10.701	1.00	46.42	CDK1
ATOM	379	CG1	ILE	112	-4.032	31.471	9.566	1.00	42.34	CDK1
ATOM	380	CD1	ILE	112	-5.506	31.301	9.436	1.00	41.68	CDK1
ATOM	381	C	ILE	112	-1.590	33.598	11.619	1.00	51.57	CDK1
ATOM	382	O	ILE	112	-1.130	34.697	11.284	1.00	49.80	CDK1
ATOM	383	N	ILE	113	-1.686	33.211	12.885	1.00	53.49	CDK1
ATOM	384	CA	ILE	113	-1.239	34.087	13.958	1.00	50.26	CDK1
ATOM	385	CB	ILE	113	-1.329	33.381	15.343	1.00	48.04	CDK1
ATOM	386	CG2	ILE	113	-0.765	34.277	16.421	1.00	46.83	CDK1
ATOM	387	CG1	ILE	113	-2.780	33.042	15.669	1.00	45.10	CDK1
ATOM	388	CD1	ILE	113	-3.666	34.248	15.756	1.00	44.59	CDK1
ATOM	389	C	ILE	113	0.212	34.450	13.670	1.00	46.14	CDK1
ATOM	390	O	ILE	113	0.609	35.611	13.789	1.00	42.78	CDK1
ATOM	391	N	ARG	114	0.990	33.446	13.273	1.00	47.90	CDK1
ATOM	392	CA	ARG	114	2.408	33.635	12.978	1.00	55.34	CDK1
ATOM	393	CB	ARG	114	3.037	32.298	12.570	1.00	63.33	CDK1
ATOM	394	CG	ARG	114	4.551	32.346	12.352	1.00	70.69	CDK1
ATOM	395	CD	ARG	114	5.065	31.070	11.662	1.00	77.06	CDK1
ATOM	396	NE	ARG	114	4.884	31.073	10.206	1.00	84.21	CDK1
ATOM	397	CZ	ARG	114	5.536	31.876	9.363	1.00	84.59	CDK1
ATOM	398	NH1	ARG	114	6.420	32.751	9.829	1.00	80.46	CDK1
ATOM	399	NH2	ARG	114	5.307	31.802	8.054	1.00	84.00	CDK1
ATOM	400	C	ARG	114	2.619	34.663	11.876	1.00	55.70	CDK1
ATOM	401	O	ARG	114	3.445	35.569	11.998	1.00	54.83	CDK1
ATOM	402	N	GLU	115	1.863	34.522	10.796	1.00	56.18	CDK1
ATOM	403	CA	GLU	115	1.990	35.443	9.681	1.00	56.04	CDK1
ATOM	404	CB	GLU	115	1.294	34.865	8.447	1.00	58.68	CDK1
ATOM	405	CG	GLU	115	2.019	33.682	7.807	1.00	55.29	CDK1
ATOM	406	CD	GLU	115	1.140	32.936	6.805	1.00	56.66	CDK1
ATOM	407	OE1	GLU	115	1.587	31.900	6.265	1.00	49.98	CDK1
ATOM	408	OE2	GLU	115	-0.001	33.390	6.560	1.00	55.37	CDK1
ATOM	409	C	GLU	115	1.405	36.814	10.018	1.00	52.31	CDK1
ATOM	410	O	GLU	115	1.859	37.833	9.496	1.00	54.38	CDK1
ATOM	411	N	LEU	116	0.403	36.836	10.894	1.00	50.32	CDK1
ATOM	412	CA	LEU	116	-0.256	38.087	11.288	1.00	45.58	CDK1
ATOM	413	CB	LEU	116	-1.478	37.786	12.145	1.00	43.27	CDK1
ATOM	414	CG	LEU	116	-2.891	37.962	11.605	1.00	46.75	CDK1
ATOM	415	CD1	LEU	116	-2.897	38.080	10.084	1.00	44.45	CDK1
ATOM	416	CD2	LEU	116	-3.712	36.762	12.070	1.00	41.67	CDK1
ATOM	417	C	LEU	116	0.673	39.017	12.055	1.00	41.14	CDK1
ATOM	418	O	LEU	116	0.396	40.200	12.185	1.00	43.42	CDK1
ATOM	419	N	GLN	117	1.781	38.478	12.551	1.00	45.96	CDK1
ATOM	420	CA	GLN	117	2.761	39.267	13.304	1.00	48.47	CDK1

ATOM	421	CB	GLN	117	3.837	38.348	13.899	1.00	51.42	CDK1
ATOM	422	CG	GLN	117	3.312	37.373	14.946	1.00	49.25	CDK1
ATOM	423	CD	GLN	117	2.231	37.995	15.818	1.00	51.87	CDK1
ATOM	424	OE1	GLN	117	1.133	37.445	15.967	1.00	49.51	CDK1
ATOM	425	NE2	GLN	117	2.537	39.153	16.392	1.00	52.38	CDK1
ATOM	426	C	GLN	117	3.426	40.344	12.453	1.00	48.67	CDK1
ATOM	427	O	GLN	117	3.954	41.332	12.979	1.00	48.37	CDK1
ATOM	428	N	VAL	118	3.413	40.153	11.137	1.00	48.39	CDK1
ATOM	429	CA	VAL	118	4.008	41.133	10.238	1.00	42.75	CDK1
ATOM	430	CB	VAL	118	3.834	40.718	8.760	1.00	48.51	CDK1
ATOM	431	CG1	VAL	118	4.494	41.756	7.851	1.00	37.54	CDK1
ATOM	432	CG2	VAL	118	4.430	39.329	8.537	1.00	46.05	CDK1
ATOM	433	C	VAL	118	3.343	42.489	10.440	1.00	38.54	CDK1
ATOM	434	O	VAL	118	3.958	43.531	10.234	1.00	39.78	CDK1
ATOM	435	N	LEU	119	2.082	42.477	10.850	1.00	38.55	CDK1
ATOM	436	CA	LEU	119	1.356	43.716	11.057	1.00	40.41	CDK1
ATOM	437	CB	LEU	119	-0.084	43.392	11.475	1.00	38.33	CDK1
ATOM	438	CG	LEU	119	-0.875	42.779	10.303	1.00	37.22	CDK1
ATOM	439	CD1	LEU	119	-2.272	42.345	10.759	1.00	37.85	CDK1
ATOM	440	CD2	LEU	119	-0.985	43.809	9.178	1.00	32.79	CDK1
ATOM	441	C	LEU	119	2.027	44.696	12.033	1.00	45.93	CDK1
ATOM	442	O	LEU	119	1.824	45.908	11.934	1.00	50.15	CDK1
ATOM	443	N	HIS	120	2.840	44.194	12.963	1.00	50.31	CDK1
ATOM	444	CA	HIS	120	3.530	45.087	13.896	1.00	52.77	CDK1
ATOM	445	CB	HIS	120	4.301	44.283	14.952	1.00	52.90	CDK1
ATOM	446	CG	HIS	120	3.467	43.870	16.127	1.00	54.80	CDK1
ATOM	447	CD2	HIS	120	2.749	44.602	17.014	1.00	51.20	CDK1
ATOM	448	ND1	HIS	120	3.297	42.548	16.494	1.00	54.79	CDK1
ATOM	449	CE1	HIS	120	2.510	42.485	17.554	1.00	53.44	CDK1
ATOM	450	NE2	HIS	120	2.163	43.717	17.889	1.00	52.87	CDK1
ATOM	451	C	HIS	120	4.507	45.972	13.117	1.00	54.96	CDK1
ATOM	452	O	HIS	120	4.824	47.082	13.536	1.00	57.39	CDK1
ATOM	453	N	GLU	121	4.969	45.470	11.975	1.00	58.29	CDK1
ATOM	454	CA	GLU	121	5.914	46.183	11.114	1.00	60.73	CDK1
ATOM	455	CB	GLU	121	6.778	45.178	10.341	1.00	65.38	CDK1
ATOM	456	CG	GLU	121	7.888	44.544	11.149	1.00	72.79	CDK1
ATOM	457	CD	GLU	121	7.585	44.512	12.634	1.00	81.01	CDK1
ATOM	458	OE1	GLU	121	7.347	43.407	13.169	1.00	85.74	CDK1
ATOM	459	OE2	GLU	121	7.587	45.592	13.266	1.00	86.07	CDK1
ATOM	460	C	GLU	121	5.271	47.155	10.112	1.00	60.03	CDK1
ATOM	461	O	GLU	121	5.983	47.905	9.437	1.00	58.90	CDK1
ATOM	462	N	CYS	122	3.943	47.146	10.004	1.00	56.14	CDK1
ATOM	463	CA	CYS	122	3.271	48.056	9.083	1.00	54.53	CDK1

ATOM	464	CB	CYS	122	2.033	47.392	8.468	1.00	50.85	CDK1
ATOM	465	SG	CYS	122	2.417	45.911	7.505	1.00	46.69	CDK1
ATOM	466	C	CYS	122	2.878	49.348	9.787	1.00	56.52	CDK1
ATOM	467	O	CYS	122	1.752	49.500	10.261	1.00	61.33	CDK1
ATOM	468	N	ASN	123	3.825	50.275	9.860	1.00	58.19	CDK1
ATOM	469	CA	ASN	123	3.590	51.569	10.494	1.00	58.56	CDK1
ATOM	470	CB	ASN	123	4.709	51.899	11.496	1.00	62.19	CDK1
ATOM	471	CG	ASN	123	5.346	50.658	12.100	1.00	67.77	CDK1
ATOM	472	OD1	ASN	123	4.655	49.778	12.613	1.00	68.61	CDK1
ATOM	473	ND2	ASN	123	6.674	50.583	12.040	1.00	72.39	CDK1
ATOM	474	C	ASN	123	3.547	52.632	9.407	1.00	54.27	CDK1
ATOM	475	O	ASN	123	4.518	52.824	8.673	1.00	55.58	CDK1
ATOM	476	N	SER	124	2.419	53.321	9.296	1.00	49.54	CDK1
ATOM	477	CA	SER	124	2.282	54.346	8.275	1.00	48.71	CDK1
ATOM	478	CB	SER	124	2.299	53.714	6.876	1.00	46.49	CDK1
ATOM	479	OG	SER	124	1.362	54.355	6.020	1.00	46.97	CDK1
ATOM	480	C	SER	124	1.002	55.141	8.439	1.00	47.55	CDK1
ATOM	481	O	SER	124	-0.065	54.583	8.669	1.00	53.05	CDK1
ATOM	482	N	PRO	125	1.094	56.464	8.304	1.00	47.17	CDK1
ATOM	483	CD	PRO	125	2.340	57.191	8.017	1.00	41.69	CDK1
ATOM	484	CA	PRO	125	-0.059	57.357	8.432	1.00	45.89	CDK1
ATOM	485	CB	PRO	125	0.426	58.669	7.829	1.00	41.81	CDK1
ATOM	486	CG	PRO	125	1.891	58.606	7.851	1.00	40.25	CDK1
ATOM	487	C	PRO	125	-1.264	56.832	7.663	1.00	47.40	CDK1
ATOM	488	O	PRO	125	-2.402	57.166	7.979	1.00	50.73	CDK1
ATOM	489	N	TYR	126	-1.003	56.013	6.648	1.00	48.48	CDK1
ATOM	490	CA	TYR	126	-2.068	55.480	5.800	1.00	47.17	CDK1
ATOM	491	CB	TYR	126	-1.642	55.612	4.336	1.00	43.20	CDK1
ATOM	492	CG	TYR	126	-1.201	57.015	4.020	1.00	38.69	CDK1
ATOM	493	CD1	TYR	126	0.147	57.340	3.915	1.00	41.99	CDK1
ATOM	494	CE1	TYR	126	0.555	58.654	3.732	1.00	42.30	CDK1
ATOM	495	CD2	TYR	126	-2.131	58.041	3.925	1.00	44.26	CDK1
ATOM	496	CE2	TYR	126	-1.734	59.354	3.742	1.00	44.20	CDK1
ATOM	497	CZ	TYR	126	-0.397	59.652	3.650	1.00	43.47	CDK1
ATOM	498	OH	TYR	126	-0.026	60.958	3.476	1.00	53.32	CDK1
ATOM	499	C	TYR	126	-2.528	54.060	6.105	1.00	46.91	CDK1
ATOM	500	O	TYR	126	-3.520	53.590	5.537	1.00	46.21	CDK1
ATOM	501	N	ILE	127	-1.824	53.387	7.011	1.00	41.71	CDK1
ATOM	502	CA	ILE	127	-2.190	52.037	7.395	1.00	38.87	CDK1
ATOM	503	CB	ILE	127	-0.989	51.077	7.352	1.00	33.27	CDK1
ATOM	504	CG2	ILE	127	-1.416	49.706	7.910	1.00	28.20	CDK1
ATOM	505	CG1	ILE	127	-0.505	50.897	5.913	1.00	34.41	CDK1
ATOM	506	CD1	ILE	127	-1.631	50.680	4.888	1.00	33.61	CDK1

ATOM	507	C	ILE	127	-2.741	52.014	8.808	1.00	38.38	CDK1
ATOM	508	O	ILE	127	-2.098	52.499	9.733	1.00	36.34	CDK1
ATOM	509	N	VAL	128	-3.926	51.442	8.973	1.00	38.31	CDK1
ATOM	510	CA	VAL	128	-4.545	51.346	10.293	1.00	40.78	CDK1
ATOM	511	CB	VAL	128	-5.912	50.606	10.212	1.00	42.58	CDK1
ATOM	512	CG1	VAL	128	-6.448	50.317	11.617	1.00	35.52	CDK1
ATOM	513	CG2	VAL	128	-6.920	51.460	9.429	1.00	33.65	CDK1
ATOM	514	C	VAL	128	-3.617	50.630	11.287	1.00	40.15	CDK1
ATOM	515	O	VAL	128	-3.220	49.483	11.075	1.00	37.55	CDK1
ATOM	516	N	GLY	129	-3.269	51.334	12.368	1.00	39.83	CDK1
ATOM	517	CA	GLY	129	-2.391	50.793	13.398	1.00	36.87	CDK1
ATOM	518	C	GLY	129	-2.884	49.468	13.932	1.00	38.58	CDK1
ATOM	519	O	GLY	129	-4.083	49.261	14.086	1.00	42.20	CDK1
ATOM	520	N	PHE	130	-1.953	48.569	14.215	1.00	35.41	CDK1
ATOM	521	CA	PHE	130	-2.287	47.246	14.703	1.00	37.73	CDK1
ATOM	522	CB	PHE	130	-1.722	46.209	13.728	1.00	36.20	CDK1
ATOM	523	CG	PHE	130	-1.503	44.825	14.318	1.00	33.41	CDK1
ATOM	524	CD1	PHE	130	-0.235	44.426	14.729	1.00	30.03	CDK1
ATOM	525	CD2	PHE	130	-2.512	43.873	14.271	1.00	27.78	CDK1
ATOM	526	CE1	PHE	130	0.033	43.090	15.059	1.00	30.52	CDK1
ATOM	527	CE2	PHE	130	-2.267	42.531	14.597	1.00	30.18	CDK1
ATOM	528	CZ	PHE	130	-0.991	42.136	14.986	1.00	32.22	CDK1
ATOM	529	C	PHE	130	-1.679	47.084	16.080	1.00	37.86	CDK1
ATOM	530	O	PHE	130	-0.579	47.590	16.334	1.00	36.91	CDK1
ATOM	531	N	TYR	131	-2.393	46.377	16.958	1.00	41.16	CDK1
ATOM	532	CA	TYR	131	-1.926	46.157	18.340	1.00	43.64	CDK1
ATOM	533	CB	TYR	131	-2.997	46.588	19.357	1.00	35.59	CDK1
ATOM	534	CG	TYR	131	-3.313	48.068	19.353	1.00	32.39	CDK1
ATOM	535	CD1	TYR	131	-2.331	49.018	19.645	1.00	41.47	CDK1
ATOM	536	CE1	TYR	131	-2.608	50.397	19.604	1.00	38.50	CDK1
ATOM	537	CD2	TYR	131	-4.583	48.520	19.031	1.00	30.65	CDK1
ATOM	538	CE2	TYR	131	-4.879	49.890	18.986	1.00	34.44	CDK1
ATOM	539	CZ	TYR	131	-3.887	50.823	19.265	1.00	42.86	CDK1
ATOM	540	OH	TYR	131	-4.170	52.180	19.133	1.00	46.26	CDK1
ATOM	541	C	TYR	131	-1.515	44.709	18.621	1.00	45.30	CDK1
ATOM	542	O	TYR	131	-0.627	44.464	19.438	1.00	53.94	CDK1
ATOM	543	N	GLY	132	-2.165	43.749	17.964	1.00	42.83	CDK1
ATOM	544	CA	GLY	132	-1.803	42.357	18.163	1.00	34.17	CDK1
ATOM	545	C	GLY	132	-2.874	41.379	17.730	1.00	38.88	CDK1
ATOM	546	O	GLY	132	-4.047	41.733	17.594	1.00	39.99	CDK1
ATOM	547	N	ALA	133	-2.465	40.132	17.525	1.00	38.56	CDK1
ATOM	548	CA	ALA	133	-3.387	39.089	17.104	1.00	39.62	CDK1
ATOM	549	CB	ALA	133	-3.179	38.764	15.622	1.00	41.73	CDK1

ATOM	550	C	ALA	133	-3.170	37.842	17.926	1.00	39.85	CDK1
ATOM	551	O	ALA	133	-2.035	37.489	18.253	1.00	40.21	CDK1
ATOM	552	N	PHE	134	-4.260	37.163	18.246	1.00	35.61	CDK1
ATOM	553	CA	PHE	134	-4.159	35.941	19.022	1.00	45.12	CDK1
ATOM	554	CB	PHE	134	-4.040	36.268	20.526	1.00	41.96	CDK1
ATOM	555	CG	PHE	134	-5.179	37.089	21.058	1.00	31.91	CDK1
ATOM	556	CD1	PHE	134	-6.351	36.482	21.475	1.00	33.97	CDK1
ATOM	557	CD2	PHE	134	-5.097	38.472	21.088	1.00	32.23	CDK1
ATOM	558	CE1	PHE	134	-7.444	37.248	21.915	1.00	36.95	CDK1
ATOM	559	CE2	PHE	134	-6.182	39.252	21.523	1.00	37.90	CDK1
ATOM	560	CZ	PHE	134	-7.362	38.634	21.937	1.00	33.70	CDK1
ATOM	561	C	PHE	134	-5.409	35.125	18.746	1.00	50.09	CDK1
ATOM	562	O	PHE	134	-6.397	35.657	18.237	1.00	52.08	CDK1
ATOM	563	N	TYR	135	-5.361	33.838	19.069	1.00	56.87	CDK1
ATOM	564	CA	TYR	135	-6.501	32.959	18.837	1.00	67.31	CDK1
ATOM	565	CB	TYR	135	-6.036	31.645	18.201	1.00	72.19	CDK1
ATOM	566	CG	TYR	135	-7.152	30.637	18.014	1.00	79.89	CDK1
ATOM	567	CD1	TYR	135	-7.135	29.411	18.685	1.00	80.25	CDK1
ATOM	568	CE1	TYR	135	-8.181	28.501	18.541	1.00	83.86	CDK1
ATOM	569	CD2	TYR	135	-8.246	30.926	17.189	1.00	82.34	CDK1
ATOM	570	CE2	TYR	135	-9.296	30.023	17.039	1.00	83.77	CDK1
ATOM	571	CZ	TYR	135	-9.259	28.814	17.717	1.00	84.64	CDK1
ATOM	572	OH	TYR	135	-10.302	27.925	17.575	1.00	86.01	CDK1
ATOM	573	C	TYR	135	-7.234	32.657	20.136	1.00	69.30	CDK1
ATOM	574	O	TYR	135	-6.649	32.088	21.058	1.00	70.72	CDK1
ATOM	575	N	SER	136	-8.513	33.019	20.209	1.00	70.59	CDK1
ATOM	576	CA	SER	136	-9.277	32.769	21.423	1.00	71.94	CDK1
ATOM	577	CB	SER	136	-9.650	34.085	22.108	1.00	72.42	CDK1
ATOM	578	OG	SER	136	-10.682	33.870	23.056	1.00	64.50	CDK1
ATOM	579	C	SER	136	-10.541	31.947	21.254	1.00	72.35	CDK1
ATOM	580	O	SER	136	-11.504	32.377	20.617	1.00	71.71	CDK1
ATOM	581	N	ASP	137	-10.519	30.765	21.856	1.00	75.45	CDK1
ATOM	582	CA	ASP	137	-11.644	29.841	21.857	1.00	78.40	CDK1
ATOM	583	CB	ASP	137	-12.505	30.085	23.107	1.00	86.60	CDK1
ATOM	584	CG	ASP	137	-11.719	29.902	24.419	1.00	94.95	CDK1
ATOM	585	OD1	ASP	137	-11.770	28.791	25.007	1.00	97.24	CDK1
ATOM	586	OD2	ASP	137	-11.055	30.872	24.862	1.00	95.41	CDK1
ATOM	587	C	ASP	137	-12.518	29.899	20.614	1.00	76.04	CDK1
ATOM	588	O	ASP	137	-13.611	30.470	20.637	1.00	75.62	CDK1
ATOM	589	N	GLY	138	-12.026	29.303	19.532	1.00	74.00	CDK1
ATOM	590	CA	GLY	138	-12.771	29.265	18.286	1.00	73.59	CDK1
ATOM	591	C	GLY	138	-12.802	30.544	17.468	1.00	75.39	CDK1
ATOM	592	O	GLY	138	-13.701	30.729	16.639	1.00	75.51	CDK1

ATOM	593	N	GLU	139	-11.830	31.428	17.673	1.00	70.82	CDK1
ATOM	594	CA	GLU	139	-11.823	32.667	16.923	1.00	66.85	CDK1
ATOM	595	CB	GLU	139	-12.924	33.584	17.429	1.00	66.45	CDK1
ATOM	596	CG	GLU	139	-13.895	33.991	16.353	1.00	72.15	CDK1
ATOM	597	CD	GLU	139	-15.318	33.613	16.697	1.00	79.37	CDK1
ATOM	598	OE1	GLU	139	-15.673	32.427	16.533	1.00	84.26	CDK1
ATOM	599	OE2	GLU	139	-16.081	34.501	17.136	1.00	83.42	CDK1
ATOM	600	C	GLU	139	-10.522	33.428	16.935	1.00	63.77	CDK1
ATOM	601	O	GLU	139	-10.111	33.954	17.965	1.00	68.67	CDK1
ATOM	602	N	ILE	140	-9.879	33.491	15.775	1.00	61.01	CDK1
ATOM	603	CA	ILE	140	-8.641	34.235	15.647	1.00	55.58	CDK1
ATOM	604	CB	ILE	140	-8.049	34.108	14.241	1.00	51.04	CDK1
ATOM	605	CG2	ILE	140	-9.093	34.471	13.199	1.00	56.56	CDK1
ATOM	606	CG1	ILE	140	-6.829	35.016	14.119	1.00	53.86	CDK1
ATOM	607	CD1	ILE	140	-7.145	36.427	13.681	1.00	52.77	CDK1
ATOM	608	C	ILE	140	-9.020	35.689	15.908	1.00	51.08	CDK1
ATOM	609	O	ILE	140	-10.060	36.158	15.446	1.00	53.47	CDK1
ATOM	610	N	SER	141	-8.171	36.397	16.640	1.00	43.43	CDK1
ATOM	611	CA	SER	141	-8.443	37.782	17.000	1.00	43.26	CDK1
ATOM	612	CB	SER	141	-8.468	37.909	18.537	1.00	44.99	CDK1
ATOM	613	OG	SER	141	-9.730	38.332	19.016	1.00	37.13	CDK1
ATOM	614	C	SER	141	-7.411	38.749	16.455	1.00	40.70	CDK1
ATOM	615	O	SER	141	-6.218	38.445	16.476	1.00	40.42	CDK1
ATOM	616	N	ILE	142	-7.873	39.914	15.987	1.00	37.09	CDK1
ATOM	617	CA	ILE	142	-6.989	40.978	15.469	1.00	39.42	CDK1
ATOM	618	CB	ILE	142	-7.058	41.116	13.891	1.00	38.19	CDK1
ATOM	619	CG2	ILE	142	-6.182	42.271	13.423	1.00	32.01	CDK1
ATOM	620	CG1	ILE	142	-6.557	39.834	13.216	1.00	44.44	CDK1
ATOM	621	CD1	ILE	142	-6.740	39.819	11.682	1.00	40.16	CDK1
ATOM	622	C	ILE	142	-7.406	42.322	16.097	1.00	36.06	CDK1
ATOM	623	O	ILE	142	-8.583	42.707	16.053	1.00	37.32	CDK1
ATOM	624	N	CYS	143	-6.443	43.044	16.659	1.00	33.42	CDK1
ATOM	625	CA	CYS	143	-6.752	44.317	17.310	1.00	33.84	CDK1
ATOM	626	CB	CYS	143	-6.402	44.227	18.800	1.00	36.04	CDK1
ATOM	627	SG	CYS	143	-6.847	42.624	19.565	1.00	43.97	CDK1
ATOM	628	C	CYS	143	-6.054	45.508	16.650	1.00	38.10	CDK1
ATOM	629	O	CYS	143	-4.819	45.527	16.420	1.00	30.00	CDK1
ATOM	630	N	MET	144	-6.858	46.519	16.356	1.00	35.26	CDK1
ATOM	631	CA	MET	144	-6.340	47.681	15.685	1.00	37.24	CDK1
ATOM	632	CB	MET	144	-6.783	47.659	14.215	1.00	41.01	CDK1
ATOM	633	CG	MET	144	-7.553	46.417	13.771	1.00	48.56	CDK1
ATOM	634	SD	MET	144	-8.778	46.771	12.467	1.00	52.36	CDK1
ATOM	635	CE	MET	144	-9.908	45.358	12.674	1.00	42.79	CDK1

ATOM	636	C	MET	144	-6.753	49.006	16.290	1.00	39.86	CDK1
ATOM	637	O	MET	144	-7.629	49.092	17.165	1.00	42.43	CDK1
ATOM	638	N	GLU	145	-6.102	50.046	15.794	1.00	38.93	CDK1
ATOM	639	CA	GLU	145	-6.408	51.397	16.197	1.00	40.38	CDK1
ATOM	640	CB	GLU	145	-5.587	52.355	15.345	1.00	38.81	CDK1
ATOM	641	CG	GLU	145	-6.237	53.671	15.000	1.00	37.85	CDK1
ATOM	642	CD	GLU	145	-5.272	54.537	14.223	1.00	41.96	CDK1
ATOM	643	OE1	GLU	145	-5.504	55.759	14.111	1.00	41.59	CDK1
ATOM	644	OE2	GLU	145	-4.264	53.980	13.725	1.00	38.99	CDK1
ATOM	645	C	GLU	145	-7.895	51.538	15.910	1.00	43.92	CDK1
ATOM	646	O	GLU	145	-8.392	51.048	14.889	1.00	47.32	CDK1
ATOM	647	N	HIS	146	-8.614	52.163	16.829	1.00	45.41	CDK1
ATOM	648	CA	HIS	146	-10.041	52.357	16.662	1.00	39.21	CDK1
ATOM	649	CB	HIS	146	-10.698	52.534	18.042	1.00	39.51	CDK1
ATOM	650	CG	HIS	146	-12.063	53.146	17.997	1.00	41.31	CDK1
ATOM	651	CD2	HIS	146	-12.475	54.418	18.207	1.00	41.75	CDK1
ATOM	652	ND1	HIS	146	-13.189	52.435	17.642	1.00	47.14	CDK1
ATOM	653	CE1	HIS	146	-14.235	53.243	17.632	1.00	41.18	CDK1
ATOM	654	NE2	HIS	146	-13.827	54.452	17.971	1.00	35.61	CDK1
ATOM	655	C	HIS	146	-10.143	53.608	15.804	1.00	38.15	CDK1
ATOM	656	O	HIS	146	-9.387	54.551	15.992	1.00	40.97	CDK1
ATOM	657	N	MET	147	-11.041	53.612	14.830	1.00	38.08	CDK1
ATOM	658	CA	MET	147	-11.166	54.776	13.972	1.00	40.67	CDK1
ATOM	659	CB	MET	147	-10.879	54.397	12.510	1.00	41.89	CDK1
ATOM	660	CG	MET	147	-9.474	53.843	12.278	1.00	32.94	CDK1
ATOM	661	SD	MET	147	-8.141	55.102	12.256	1.00	40.39	CDK1
ATOM	662	CE	MET	147	-8.881	56.336	11.082	1.00	33.20	CDK1
ATOM	663	C	MET	147	-12.558	55.354	14.127	1.00	44.96	CDK1
ATOM	664	O	MET	147	-13.517	54.897	13.514	1.00	44.70	CDK1
ATOM	665	N	ASP	148	-12.640	56.378	14.962	1.00	49.75	CDK1
ATOM	666	CA	ASP	148	-13.891	57.043	15.290	1.00	53.81	CDK1
ATOM	667	CB	ASP	148	-13.617	58.150	16.315	1.00	62.08	CDK1
ATOM	668	CG	ASP	148	-12.709	59.236	15.779	1.00	64.51	CDK1
ATOM	669	OD1	ASP	148	-12.651	60.311	16.407	1.00	65.57	CDK1
ATOM	670	OD2	ASP	148	-12.059	59.016	14.736	1.00	66.33	CDK1
ATOM	671	C	ASP	148	-14.705	57.604	14.136	1.00	53.89	CDK1
ATOM	672	O	ASP	148	-15.893	57.883	14.299	1.00	54.66	CDK1
ATOM	673	N	GLY	149	-14.077	57.785	12.980	1.00	56.00	CDK1
ATOM	674	CA	GLY	149	-14.795	58.306	11.834	1.00	50.16	CDK1
ATOM	675	C	GLY	149	-15.542	57.185	11.138	1.00	50.14	CDK1
ATOM	676	O	GLY	149	-16.547	57.413	10.473	1.00	47.39	CDK1
ATOM	677	N	GLY	150	-15.053	55.960	11.309	1.00	49.29	CDK1
ATOM	678	CA	GLY	150	-15.682	54.818	10.670	1.00	49.79	CDK1

ATOM	679	C	GLY	150	-15.095	54.483	9.300	1.00	47.68	CDK1
ATOM	680	O	GLY	150	-13.989	54.919	8.946	1.00	46.35	CDK1
ATOM	681	N	SER	151	-15.840	53.692	8.535	1.00	43.32	CDK1
ATOM	682	CA	SER	151	-15.417	53.279	7.203	1.00	45.70	CDK1
ATOM	683	CB	SER	151	-15.704	51.800	6.998	1.00	42.39	CDK1
ATOM	684	OG	SER	151	-17.062	51.527	7.290	1.00	43.65	CDK1
ATOM	685	C	SER	151	-16.206	54.099	6.198	1.00	48.52	CDK1
ATOM	686	O	SER	151	-17.396	54.372	6.407	1.00	48.08	CDK1
ATOM	687	N	LEU	152	-15.556	54.469	5.099	1.00	46.59	CDK1
ATOM	688	CA	LEU	152	-16.195	55.301	4.088	1.00	44.86	CDK1
ATOM	689	CB	LEU	152	-15.234	55.558	2.927	1.00	39.28	CDK1
ATOM	690	CG	LEU	152	-14.068	56.504	3.268	1.00	40.54	CDK1
ATOM	691	CD1	LEU	152	-13.277	56.863	2.006	1.00	40.41	CDK1
ATOM	692	CD2	LEU	152	-14.604	57.766	3.938	1.00	41.33	CDK1
ATOM	693	C	LEU	152	-17.547	54.844	3.567	1.00	43.60	CDK1
ATOM	694	O	LEU	152	-18.313	55.664	3.086	1.00	44.81	CDK1
ATOM	695	N	ASP	153	-17.866	53.559	3.653	1.00	46.08	CDK1
ATOM	696	CA	ASP	153	-19.186	53.136	3.186	1.00	49.64	CDK1
ATOM	697	CB	ASP	153	-19.321	51.610	3.163	1.00	51.94	CDK1
ATOM	698	CG	ASP	153	-19.096	50.987	4.517	1.00	57.34	CDK1
ATOM	699	OD1	ASP	153	-20.000	50.271	5.005	1.00	58.71	CDK1
ATOM	700	OD2	ASP	153	-18.010	51.215	5.089	1.00	59.88	CDK1
ATOM	701	C	ASP	153	-20.232	53.740	4.124	1.00	50.52	CDK1
ATOM	702	O	ASP	153	-21.318	54.126	3.694	1.00	51.30	CDK1
ATOM	703	N	GLN	154	-19.906	53.829	5.408	1.00	51.16	CDK1
ATOM	704	CA	GLN	154	-20.837	54.429	6.356	1.00	54.80	CDK1
ATOM	705	CB	GLN	154	-20.371	54.198	7.805	1.00	55.16	CDK1
ATOM	706	CG	GLN	154	-19.538	52.934	8.033	1.00	60.53	CDK1
ATOM	707	CD	GLN	154	-19.219	52.682	9.510	1.00	62.13	CDK1
ATOM	708	OE1	GLN	154	-18.057	52.735	9.943	1.00	56.52	CDK1
ATOM	709	NE2	GLN	154	-20.253	52.401	10.286	1.00	63.87	CDK1
ATOM	710	C	GLN	154	-20.917	55.936	6.053	1.00	53.44	CDK1
ATOM	711	O	GLN	154	-22.003	56.487	5.870	1.00	52.56	CDK1
ATOM	712	N	VAL	155	-19.759	56.590	5.985	1.00	52.33	CDK1
ATOM	713	CA	VAL	155	-19.693	58.021	5.694	1.00	48.04	CDK1
ATOM	714	CB	VAL	155	-18.222	58.486	5.561	1.00	45.68	CDK1
ATOM	715	CG1	VAL	155	-18.152	59.966	5.215	1.00	38.72	CDK1
ATOM	716	CG2	VAL	155	-17.483	58.209	6.855	1.00	31.90	CDK1
ATOM	717	C	VAL	155	-20.453	58.365	4.410	1.00	53.41	CDK1
ATOM	718	O	VAL	155	-21.019	59.446	4.284	1.00	56.08	CDK1
ATOM	719	N	LEU	156	-20.471	57.438	3.458	1.00	56.29	CDK1
ATOM	720	CA	LEU	156	-21.170	57.650	2.195	1.00	53.42	CDK1
ATOM	721	CB	LEU	156	-20.717	56.616	1.161	1.00	54.21	CDK1

ATOM	722	CG	LEU	156	-20.961	56.868	-0.334	1.00	52.87	CDK1
ATOM	723	CD1	LEU	156	-22.332	56.373	-0.697	1.00	54.42	CDK1
ATOM	724	CD2	LEU	156	-20.815	58.343	-0.665	1.00	49.22	CDK1
ATOM	725	C	LEU	156	-22.677	57.547	2.381	1.00	53.72	CDK1
ATOM	726	O	LEU	156	-23.434	58.259	1.726	1.00	58.13	CDK1
ATOM	727	N	ALA	157	-23.118	56.653	3.262	1.00	51.68	CDK1
ATOM	728	CA	ALA	157	-24.547	56.485	3.507	1.00	52.70	CDK1
ATOM	729	CB	ALA	157	-24.807	55.270	4.391	1.00	44.13	CDK1
ATOM	730	C	ALA	157	-25.080	57.745	4.172	1.00	57.46	CDK1
ATOM	731	O	ALA	157	-26.151	58.244	3.809	1.00	62.34	CDK1
ATOM	732	N	ALA	158	-24.322	58.269	5.133	1.00	59.17	CDK1
ATOM	733	CA	ALA	158	-24.718	59.477	5.846	1.00	59.90	CDK1
ATOM	734	CB	ALA	158	-24.165	59.451	7.274	1.00	52.49	CDK1
ATOM	735	C	ALA	158	-24.252	60.739	5.125	1.00	63.87	CDK1
ATOM	736	O	ALA	158	-24.166	61.803	5.729	1.00	67.93	CDK1
ATOM	737	N	ALA	159	-23.953	60.624	3.833	1.00	68.87	CDK1
ATOM	738	CA	ALA	159	-23.496	61.777	3.053	1.00	68.84	CDK1
ATOM	739	CB	ALA	159	-21.968	61.883	3.108	1.00	71.09	CDK1
ATOM	740	C	ALA	159	-23.946	61.740	1.600	1.00	70.75	CDK1
ATOM	741	O	ALA	159	-23.514	62.572	0.803	1.00	74.10	CDK1
ATOM	742	N	GLY	160	-24.800	60.779	1.255	1.00	69.95	CDK1
ATOM	743	CA	GLY	160	-25.281	60.666	-0.115	1.00	70.09	CDK1
ATOM	744	C	GLY	160	-24.153	60.379	-1.090	1.00	70.08	CDK1
ATOM	745	O	GLY	160	-23.952	59.234	-1.505	1.00	68.88	CDK1
ATOM	746	N	ARG	161	-23.428	61.432	-1.465	1.00	68.91	CDK1
ATOM	747	CA	ARG	161	-22.286	61.322	-2.365	1.00	67.50	CDK1
ATOM	748	CB	ARG	161	-22.665	61.761	-3.788	1.00	68.34	CDK1
ATOM	749	CG	ARG	161	-22.596	63.247	-4.040	1.00	69.19	CDK1
ATOM	750	CD	ARG	161	-23.933	63.770	-4.534	1.00	78.96	CDK1
ATOM	751	NE	ARG	161	-24.028	63.775	-5.991	1.00	84.58	CDK1
ATOM	752	CZ	ARG	161	-23.845	64.853	-6.754	1.00	89.53	CDK1
ATOM	753	NH1	ARG	161	-23.555	66.029	-6.201	1.00	86.18	CDK1
ATOM	754	NH2	ARG	161	-23.949	64.753	-8.076	1.00	88.45	CDK1
ATOM	755	C	ARG	161	-21.196	62.214	-1.792	1.00	62.65	CDK1
ATOM	756	O	ARG	161	-21.469	63.331	-1.368	1.00	65.06	CDK1
ATOM	757	N	ILE	162	-19.971	61.708	-1.742	1.00	59.14	CDK1
ATOM	758	CA	ILE	162	-18.864	62.486	-1.213	1.00	54.59	CDK1
ATOM	759	CB	ILE	162	-17.758	61.548	-0.691	1.00	49.92	CDK1
ATOM	760	CG2	ILE	162	-16.467	62.296	-0.491	1.00	47.22	CDK1
ATOM	761	CG1	ILE	162	-18.204	60.956	0.655	1.00	48.38	CDK1
ATOM	762	CD1	ILE	162	-17.453	59.710	1.087	1.00	44.55	CDK1
ATOM	763	C	ILE	162	-18.360	63.413	-2.320	1.00	58.76	CDK1
ATOM	764	O	ILE	162	-18.345	63.044	-3.487	1.00	60.70	CDK1

ATOM	765	N	PRO	163	-17.981	64.651	-1.966	1.00	60.66	CDK1
ATOM	766	CD	PRO	163	-18.024	65.170	-0.591	1.00	62.92	CDK1
ATOM	767	CA	PRO	163	-17.481	65.660	-2.911	1.00	58.60	CDK1
ATOM	768	CB	PRO	163	-17.481	66.959	-2.106	1.00	57.75	CDK1
ATOM	769	CG	PRO	163	-18.152	66.639	-0.799	1.00	60.35	CDK1
ATOM	770	C	PRO	163	-16.110	65.384	-3.506	1.00	58.01	CDK1
ATOM	771	O	PRO	163	-15.216	64.852	-2.842	1.00	61.16	CDK1
ATOM	772	N	GLU	164	-15.952	65.779	-4.763	1.00	55.56	CDK1
ATOM	773	CA	GLU	164	-14.713	65.580	-5.489	1.00	59.06	CDK1
ATOM	774	CB	GLU	164	-14.782	66.292	-6.835	1.00	58.49	CDK1
ATOM	775	CG	GLU	164	-13.539	66.116	-7.652	1.00	59.06	CDK1
ATOM	776	CD	GLU	164	-13.612	66.834	-8.972	1.00	61.77	CDK1
ATOM	777	OE1	GLU	164	-14.702	67.339	-9.322	1.00	66.13	CDK1
ATOM	778	OE2	GLU	164	-12.571	66.891	-9.657	1.00	61.75	CDK1
ATOM	779	C	GLU	164	-13.468	66.034	-4.736	1.00	59.68	CDK1
ATOM	780	O	GLU	164	-12.444	65.357	-4.754	1.00	64.02	CDK1
ATOM	781	N	GLN	165	-13.546	67.177	-4.072	1.00	59.85	CDK1
ATOM	782	CA	GLN	165	-12.391	67.675	-3.343	1.00	60.52	CDK1
ATOM	783	CB	GLN	165	-12.705	69.046	-2.745	1.00	62.75	CDK1
ATOM	784	CG	GLN	165	-11.621	70.077	-2.990	1.00	66.27	CDK1
ATOM	785	CD	GLN	165	-11.964	71.017	-4.127	1.00	72.52	CDK1
ATOM	786	OE1	GLN	165	-12.968	71.731	-4.075	1.00	70.95	CDK1
ATOM	787	NE2	GLN	165	-11.132	71.022	-5.167	1.00	71.27	CDK1
ATOM	788	C	GLN	165	-11.955	66.698	-2.251	1.00	59.33	CDK1
ATOM	789	O	GLN	165	-10.762	66.431	-2.078	1.00	59.08	CDK1
ATOM	790	N	ILE	166	-12.926	66.161	-1.521	1.00	57.69	CDK1
ATOM	791	CA	ILE	166	-12.637	65.210	-0.457	1.00	58.51	CDK1
ATOM	792	CB	ILE	166	-13.856	65.059	0.476	1.00	60.75	CDK1
ATOM	793	CG2	ILE	166	-13.856	63.703	1.160	1.00	64.06	CDK1
ATOM	794	CG1	ILE	166	-13.802	66.148	1.543	1.00	58.23	CDK1
ATOM	795	CD1	ILE	166	-15.071	66.913	1.660	1.00	62.11	CDK1
ATOM	796	C	ILE	166	-12.222	63.860	-1.058	1.00	55.32	CDK1
ATOM	797	O	ILE	166	-11.289	63.208	-0.578	1.00	51.78	CDK1
ATOM	798	N	LEU	167	-12.900	63.444	-2.120	1.00	56.45	CDK1
ATOM	799	CA	LEU	167	-12.531	62.198	-2.772	1.00	53.31	CDK1
ATOM	800	CB	LEU	167	-13.457	61.924	-3.956	1.00	51.32	CDK1
ATOM	801	CG	LEU	167	-14.835	61.419	-3.520	1.00	50.35	CDK1
ATOM	802	CD1	LEU	167	-15.623	60.902	-4.736	1.00	44.19	CDK1
ATOM	803	CD2	LEU	167	-14.641	60.327	-2.459	1.00	43.10	CDK1
ATOM	804	C	LEU	167	-11.087	62.334	-3.243	1.00	53.82	CDK1
ATOM	805	O	LEU	167	-10.396	61.339	-3.457	1.00	55.98	CDK1
ATOM	806	N	GLY	168	-10.633	63.579	-3.391	1.00	55.85	CDK1
ATOM	807	CA	GLY	168	-9.270	63.831	-3.821	1.00	53.39	CDK1

ATOM	808	C	GLY	168	-8.280	63.485	-2.723	1.00	53.65	CDK1
ATOM	809	O	GLY	168	-7.228	62.896	-2.980	1.00	54.15	CDK1
ATOM	810	N	ALA	169	-8.616	63.855	-1.491	1.00	54.79	CDK1
ATOM	811	CA	ALA	169	-7.753	63.562	-0.352	1.00	54.11	CDK1
ATOM	812	CB	ALA	169	-8.222	64.326	0.880	1.00	50.78	CDK1
ATOM	813	C	ALA	169	-7.756	62.052	-0.085	1.00	55.44	CDK1
ATOM	814	O	ALA	169	-6.724	61.477	0.288	1.00	58.90	CDK1
ATOM	815	N	VAL	170	-8.909	61.412	-0.294	1.00	52.10	CDK1
ATOM	816	CA	VAL	170	-9.036	59.967	-0.088	1.00	43.11	CDK1
ATOM	817	CB	VAL	170	-10.477	59.486	-0.368	1.00	42.20	CDK1
ATOM	818	CG1	VAL	170	-10.552	57.948	-0.279	1.00	38.19	CDK1
ATOM	819	CG2	VAL	170	-11.437	60.129	0.632	1.00	37.74	CDK1
ATOM	820	C	VAL	170	-8.080	59.240	-1.027	1.00	44.85	CDK1
ATOM	821	O	VAL	170	-7.342	58.331	-0.619	1.00	44.80	CDK1
ATOM	822	N	SER	171	-8.092	59.662	-2.287	1.00	43.55	CDK1
ATOM	823	CA	SER	171	-7.231	59.070	-3.298	1.00	40.59	CDK1
ATOM	824	CB	SER	171	-7.442	59.767	-4.643	1.00	43.06	CDK1
ATOM	825	OG	SER	171	-8.791	59.652	-5.069	1.00	42.32	CDK1
ATOM	826	C	SER	171	-5.774	59.159	-2.859	1.00	40.31	CDK1
ATOM	827	O	SER	171	-5.069	58.158	-2.864	1.00	44.03	CDK1
ATOM	828	N	ILE	172	-5.321	60.346	-2.469	1.00	40.37	CDK1
ATOM	829	CA	ILE	172	-3.946	60.498	-2.007	1.00	41.03	CDK1
ATOM	830	CB	ILE	172	-3.696	61.931	-1.460	1.00	41.58	CDK1
ATOM	831	CG2	ILE	172	-2.467	61.957	-0.572	1.00	46.32	CDK1
ATOM	832	CG1	ILE	172	-3.430	62.880	-2.620	1.00	47.24	CDK1
ATOM	833	CD1	ILE	172	-4.261	64.126	-2.594	1.00	54.48	CDK1
ATOM	834	C	ILE	172	-3.649	59.454	-0.915	1.00	41.13	CDK1
ATOM	835	O	ILE	172	-2.616	58.779	-0.955	1.00	39.77	CDK1
ATOM	836	N	ALA	173	-4.573	59.302	0.036	1.00	38.74	CDK1
ATOM	837	CA	ALA	173	-4.412	58.335	1.131	1.00	38.83	CDK1
ATOM	838	CB	ALA	173	-5.558	58.481	2.132	1.00	41.99	CDK1
ATOM	839	C	ALA	173	-4.340	56.890	0.654	1.00	37.38	CDK1
ATOM	840	O	ALA	173	-3.430	56.150	1.044	1.00	35.37	CDK1
ATOM	841	N	VAL	174	-5.308	56.487	-0.171	1.00	36.64	CDK1
ATOM	842	CA	VAL	174	-5.344	55.120	-0.699	1.00	38.40	CDK1
ATOM	843	CB	VAL	174	-6.551	54.875	-1.671	1.00	37.46	CDK1
ATOM	844	CG1	VAL	174	-6.410	53.519	-2.360	1.00	28.72	CDK1
ATOM	845	CG2	VAL	174	-7.855	54.928	-0.924	1.00	31.19	CDK1
ATOM	846	C	VAL	174	-4.059	54.805	-1.455	1.00	40.23	CDK1
ATOM	847	O	VAL	174	-3.452	53.761	-1.236	1.00	46.99	CDK1
ATOM	848	N	ILE	175	-3.639	55.699	-2.342	1.00	42.47	CDK1
ATOM	849	CA	ILE	175	-2.419	55.451	-3.102	1.00	45.02	CDK1
ATOM	850	CB	ILE	175	-2.269	56.430	-4.294	1.00	48.70	CDK1

ATOM	851	CG2	ILE	175	-2.681	57.803	-3.892	1.00	54.62	CDK1
ATOM	852	CG1	ILE	175	-0.817	56.467	-4.763	1.00	55.56	CDK1
ATOM	853	CD1	ILE	175	-0.525	55.540	-5.936	1.00	64.48	CDK1
ATOM	854	C	ILE	175	-1.160	55.492	-2.230	1.00	44.48	CDK1
ATOM	855	O	ILE	175	-0.324	54.608	-2.339	1.00	44.80	CDK1
ATOM	856	N	LYS	176	-1.009	56.493	-1.367	1.00	42.50	CDK1
ATOM	857	CA	LYS	176	0.178	56.523	-0.507	1.00	45.31	CDK1
ATOM	858	CB	LYS	176	0.134	57.725	0.433	1.00	47.45	CDK1
ATOM	859	CG	LYS	176	0.087	59.058	-0.301	1.00	50.22	CDK1
ATOM	860	CD	LYS	176	1.436	59.740	-0.332	1.00	48.08	CDK1
ATOM	861	CE	LYS	176	1.497	60.877	0.677	1.00	58.33	CDK1
ATOM	862	NZ	LYS	176	1.590	62.216	0.028	1.00	54.23	CDK1
ATOM	863	C	LYS	176	0.206	55.228	0.305	1.00	42.53	CDK1
ATOM	864	O	LYS	176	1.269	54.685	0.621	1.00	40.95	CDK1
ATOM	865	N	GLY	177	-0.988	54.734	0.623	1.00	41.24	CDK1
ATOM	866	CA	GLY	177	-1.119	53.498	1.376	1.00	37.73	CDK1
ATOM	867	C	GLY	177	-0.709	52.247	0.615	1.00	37.54	CDK1
ATOM	868	O	GLY	177	0.126	51.462	1.085	1.00	35.90	CDK1
ATOM	869	N	LEU	178	-1.296	52.042	-0.562	1.00	36.51	CDK1
ATOM	870	CA	LEU	178	-0.953	50.871	-1.362	1.00	34.24	CDK1
ATOM	871	CB	LEU	178	-1.815	50.822	-2.624	1.00	29.21	CDK1
ATOM	872	CG	LEU	178	-3.275	50.496	-2.338	1.00	27.26	CDK1
ATOM	873	CD1	LEU	178	-4.184	51.131	-3.365	1.00	36.36	CDK1
ATOM	874	CD2	LEU	178	-3.435	49.013	-2.356	1.00	36.72	CDK1
ATOM	875	C	LEU	178	0.532	50.839	-1.727	1.00	35.27	CDK1
ATOM	876	O	LEU	178	1.140	49.761	-1.735	1.00	37.41	CDK1
ATOM	877	N	THR	179	1.142	51.999	-1.994	1.00	41.48	CDK1
ATOM	878	CA	THR	179	2.560	51.980	-2.363	1.00	43.74	CDK1
ATOM	879	CB	THR	179	3.012	53.280	-3.130	1.00	40.51	CDK1
ATOM	880	OG1	THR	179	4.219	53.799	-2.565	1.00	45.88	CDK1
ATOM	881	CG2	THR	179	1.967	54.326	-3.094	1.00	40.22	CDK1
ATOM	882	C	THR	179	3.476	51.679	-1.175	1.00	46.52	CDK1
ATOM	883	O	THR	179	4.564	51.110	-1.355	1.00	44.65	CDK1
ATOM	884	N	TYR	180	3.037	52.033	0.036	1.00	47.42	CDK1
ATOM	885	CA	TYR	180	3.831	51.728	1.225	1.00	40.45	CDK1
ATOM	886	CB	TYR	180	3.250	52.395	2.474	1.00	45.09	CDK1
ATOM	887	CG	TYR	180	3.801	51.801	3.753	1.00	46.20	CDK1
ATOM	888	CD1	TYR	180	4.989	52.271	4.308	1.00	43.87	CDK1
ATOM	889	CE1	TYR	180	5.537	51.676	5.434	1.00	46.15	CDK1
ATOM	890	CD2	TYR	180	3.172	50.718	4.366	1.00	45.97	CDK1
ATOM	891	CE2	TYR	180	3.714	50.118	5.492	1.00	51.36	CDK1
ATOM	892	CZ	TYR	180	4.896	50.600	6.019	1.00	50.17	CDK1
ATOM	893	OH	TYR	180	5.428	50.000	7.132	1.00	55.71	CDK1

ATOM	894	C	TYR	180	3.821	50.214	1.422	1.00	40.28	CDK1
ATOM	895	O	TYR	180	4.867	49.595	1.621	1.00	39.98	CDK1
ATOM	896	N	LEU	181	2.632	49.619	1.352	1.00	39.91	CDK1
ATOM	897	CA	LEU	181	2.492	48.180	1.533	1.00	42.05	CDK1
ATOM	898	CB	LEU	181	1.010	47.772	1.450	1.00	44.75	CDK1
ATOM	899	CG	LEU	181	0.083	48.026	2.653	1.00	44.42	CDK1
ATOM	900	CD1	LEU	181	-1.349	47.791	2.231	1.00	32.18	CDK1
ATOM	901	CD2	LEU	181	0.440	47.098	3.810	1.00	38.81	CDK1
ATOM	902	C	LEU	181	3.302	47.428	0.482	1.00	47.62	CDK1
ATOM	903	O	LEU	181	4.030	46.479	0.795	1.00	49.55	CDK1
ATOM	904	N	ARG	182	3.176	47.859	-0.770	1.00	47.07	CDK1
ATOM	905	CA	ARG	182	3.892	47.227	-1.870	1.00	50.18	CDK1
ATOM	906	CB	ARG	182	3.309	47.737	-3.211	1.00	54.86	CDK1
ATOM	907	CG	ARG	182	4.281	47.859	-4.371	1.00	52.58	CDK1
ATOM	908	CD	ARG	182	3.802	47.097	-5.589	1.00	61.35	CDK1
ATOM	909	NE	ARG	182	4.836	46.171	-6.035	1.00	67.08	CDK1
ATOM	910	CZ	ARG	182	5.085	44.994	-5.467	1.00	70.86	CDK1
ATOM	911	NH1	ARG	182	4.369	44.586	-4.425	1.00	74.99	CDK1
ATOM	912	NH2	ARG	182	6.080	44.241	-5.914	1.00	71.22	CDK1
ATOM	913	C	ARG	182	5.418	47.446	-1.795	1.00	52.73	CDK1
ATOM	914	O	ARG	182	6.201	46.489	-1.910	1.00	48.17	CDK1
ATOM	915	N	GLU	183	5.843	48.688	-1.575	1.00	51.47	CDK1
ATOM	916	CA	GLU	183	7.268	48.989	-1.508	1.00	55.51	CDK1
ATOM	917	CB	GLU	183	7.486	50.494	-1.681	1.00	62.91	CDK1
ATOM	918	CG	GLU	183	8.020	50.908	-3.056	1.00	70.81	CDK1
ATOM	919	CD	GLU	183	7.497	52.270	-3.509	1.00	77.75	CDK1
ATOM	920	OE1	GLU	183	6.875	52.335	-4.595	1.00	82.33	CDK1
ATOM	921	OE2	GLU	183	7.709	53.273	-2.785	1.00	78.81	CDK1
ATOM	922	C	GLU	183	7.937	48.517	-0.213	1.00	59.74	CDK1
ATOM	923	O	GLU	183	9.015	47.920	-0.237	1.00	60.73	CDK1
ATOM	924	N	LYS	184	7.294	48.768	0.920	1.00	58.07	CDK1
ATOM	925	CA	LYS	184	7.871	48.378	2.190	1.00	54.98	CDK1
ATOM	926	CB	LYS	184	7.348	49.300	3.284	1.00	54.68	CDK1
ATOM	927	CG	LYS	184	7.746	50.753	3.079	1.00	57.51	CDK1
ATOM	928	CD	LYS	184	9.208	50.876	2.666	1.00	61.42	CDK1
ATOM	929	CE	LYS	184	9.803	52.202	3.104	1.00	61.67	CDK1
ATOM	930	NZ	LYS	184	8.938	53.338	2.671	1.00	64.63	CDK1
ATOM	931	C	LYS	184	7.655	46.931	2.590	1.00	54.22	CDK1
ATOM	932	O	LYS	184	8.455	46.380	3.332	1.00	57.79	CDK1
ATOM	933	N	HIS	185	6.595	46.300	2.099	1.00	56.92	CDK1
ATOM	934	CA	HIS	185	6.320	44.913	2.476	1.00	52.80	CDK1
ATOM	935	CB	HIS	185	5.154	44.897	3.468	1.00	52.24	CDK1
ATOM	936	CG	HIS	185	5.409	45.733	4.685	1.00	54.70	CDK1

ATOM	937	CD2	HIS	185	5.065	47.012	4.974	1.00	53.43	CDK1
ATOM	938	ND1	HIS	185	6.203	45.302	5.730	1.00	48.34	CDK1
ATOM	939	CE1	HIS	185	6.340	46.283	6.604	1.00	43.18	CDK1
ATOM	940	NE2	HIS	185	5.661	47.331	6.171	1.00	43.20	CDK1
ATOM	941	C	HIS	185	6.076	43.945	1.319	1.00	50.76	CDK1
ATOM	942	O	HIS	185	5.792	42.768	1.515	1.00	47.19	CDK1
ATOM	943	N	LYS	186	6.202	44.445	0.103	1.00	53.16	CDK1
ATOM	944	CA	LYS	186	6.028	43.609	-1.071	1.00	48.89	CDK1
ATOM	945	CB	LYS	186	7.193	42.617	-1.170	1.00	50.41	CDK1
ATOM	946	CG	LYS	186	8.585	43.272	-1.218	1.00	59.45	CDK1
ATOM	947	CD	LYS	186	9.666	42.343	-1.798	1.00	59.65	CDK1
ATOM	948	CE	LYS	186	10.692	43.118	-2.630	1.00	66.06	CDK1
ATOM	949	NZ	LYS	186	11.624	43.951	-1.804	1.00	64.91	CDK1
ATOM	950	C	LYS	186	4.719	42.845	-1.080	1.00	46.84	CDK1
ATOM	951	O	LYS	186	4.716	41.655	-1.377	1.00	50.01	CDK1
ATOM	952	N	ILE	187	3.606	43.508	-0.767	1.00	45.68	CDK1
ATOM	953	CA	ILE	187	2.310	42.822	-0.774	1.00	45.75	CDK1
ATOM	954	CB	ILE	187	1.892	42.305	0.657	1.00	50.41	CDK1
ATOM	955	CG2	ILE	187	3.102	41.811	1.426	1.00	46.80	CDK1
ATOM	956	CG1	ILE	187	1.202	43.412	1.462	1.00	48.16	CDK1
ATOM	957	CD1	ILE	187	2.076	44.602	1.738	1.00	52.11	CDK1
ATOM	958	C	ILE	187	1.181	43.695	-1.316	1.00	47.21	CDK1
ATOM	959	O	ILE	187	1.229	44.923	-1.204	1.00	43.79	CDK1
ATOM	960	N	MET	188	0.178	43.058	-1.922	1.00	44.08	CDK1
ATOM	961	CA	MET	188	-0.965	43.790	-2.440	1.00	37.55	CDK1
ATOM	962	CB	MET	188	-1.431	43.207	-3.787	1.00	41.80	CDK1
ATOM	963	CG	MET	188	-1.940	41.766	-3.764	1.00	39.96	CDK1
ATOM	964	SD	MET	188	-2.830	41.217	-5.313	1.00	38.86	CDK1
ATOM	965	CE	MET	188	-4.083	42.543	-5.537	1.00	21.07	CDK1
ATOM	966	C	MET	188	-2.106	43.768	-1.422	1.00	40.19	CDK1
ATOM	967	O	MET	188	-2.205	42.888	-0.570	1.00	39.18	CDK1
ATOM	968	N	HIS	189	-2.974	44.753	-1.497	1.00	37.84	CDK1
ATOM	969	CA	HIS	189	-4.076	44.805	-0.572	1.00	34.00	CDK1
ATOM	970	CB	HIS	189	-4.825	46.102	-0.766	1.00	30.23	CDK1
ATOM	971	CG	HIS	189	-5.719	46.430	0.375	1.00	42.70	CDK1
ATOM	972	CD2	HIS	189	-5.657	47.412	1.304	1.00	30.70	CDK1
ATOM	973	ND1	HIS	189	-6.861	45.706	0.648	1.00	45.65	CDK1
ATOM	974	CE1	HIS	189	-7.469	46.233	1.695	1.00	34.17	CDK1
ATOM	975	NE2	HIS	189	-6.758	47.269	2.110	1.00	42.24	CDK1
ATOM	976	C	HIS	189	-5.004	43.614	-0.782	1.00	36.63	CDK1
ATOM	977	O	HIS	189	-5.089	42.717	0.061	1.00	35.98	CDK1
ATOM	978	N	ARG	190	-5.678	43.610	-1.928	1.00	28.20	CDK1
ATOM	979	CA	ARG	190	-6.580	42.553	-2.329	1.00	21.48	CDK1

ATOM	980	CB	ARG	190	-6.123	41.200	-1.822	1.00	13.57	CDK1
ATOM	981	CG	ARG	190	-4.692	40.943	-2.188	1.00	32.55	CDK1
ATOM	982	CD	ARG	190	-4.148	39.748	-1.465	1.00	44.90	CDK1
ATOM	983	NE	ARG	190	-4.208	38.578	-2.321	1.00	49.78	CDK1
ATOM	984	CZ	ARG	190	-5.349	38.020	-2.702	1.00	59.03	CDK1
ATOM	985	NH1	ARG	190	-6.497	38.537	-2.293	1.00	65.18	CDK1
ATOM	986	NH2	ARG	190	-5.349	36.953	-3.488	1.00	61.12	CDK1
ATOM	987	C	ARG	190	-7.982	42.747	-1.920	1.00	23.83	CDK1
ATOM	988	O	ARG	190	-8.794	41.898	-2.206	1.00	27.41	CDK1
ATOM	989	N	ASP	191	-8.290	43.855	-1.255	1.00	32.32	CDK1
ATOM	990	CA	ASP	191	-9.666	44.072	-0.818	1.00	29.82	CDK1
ATOM	991	CB	ASP	191	-9.968	43.220	0.425	1.00	30.20	CDK1
ATOM	992	CG	ASP	191	-11.481	43.067	0.704	1.00	38.26	CDK1
ATOM	993	OD1	ASP	191	-12.316	43.358	-0.186	1.00	40.42	CDK1
ATOM	994	OD2	ASP	191	-11.837	42.650	1.835	1.00	45.82	CDK1
ATOM	995	C	ASP	191	-9.975	45.530	-0.535	1.00	31.17	CDK1
ATOM	996	O	ASP	191	-10.562	45.861	0.493	1.00	34.44	CDK1
ATOM	997	N	VAL	192	-9.590	46.415	-1.450	1.00	29.26	CDK1
ATOM	998	CA	VAL	192	-9.903	47.802	-1.232	1.00	31.21	CDK1
ATOM	999	CB	VAL	192	-8.873	48.771	-1.897	1.00	31.12	CDK1
ATOM	1000	CG1	VAL	192	-7.788	47.990	-2.595	1.00	33.67	CDK1
ATOM	1001	CG2	VAL	192	-9.570	49.759	-2.807	1.00	31.38	CDK1
ATOM	1002	C	VAL	192	-11.310	48.062	-1.707	1.00	33.82	CDK1
ATOM	1003	O	VAL	192	-11.728	47.574	-2.749	1.00	39.89	CDK1
ATOM	1004	N	LYS	193	-12.052	48.795	-0.883	1.00	38.91	CDK1
ATOM	1005	CA	LYS	193	-13.431	49.180	-1.142	1.00	33.59	CDK1
ATOM	1006	CB	LYS	193	-14.346	47.979	-1.059	1.00	32.79	CDK1
ATOM	1007	CG	LYS	193	-13.974	46.971	-0.004	1.00	36.22	CDK1
ATOM	1008	CD	LYS	193	-15.133	46.016	0.219	1.00	27.48	CDK1
ATOM	1009	CE	LYS	193	-14.625	44.664	0.607	1.00	37.64	CDK1
ATOM	1010	NZ	LYS	193	-15.537	43.986	1.570	1.00	37.76	CDK1
ATOM	1011	C	LYS	193	-13.754	50.167	-0.044	1.00	36.43	CDK1
ATOM	1012	O	LYS	193	-13.041	50.235	0.935	1.00	40.61	CDK1
ATOM	1013	N	PRO	194	-14.840	50.932	-0.175	1.00	37.75	CDK1
ATOM	1014	CD	PRO	194	-15.848	50.913	-1.249	1.00	36.30	CDK1
ATOM	1015	CA	PRO	194	-15.166	51.907	0.875	1.00	38.77	CDK1
ATOM	1016	CB	PRO	194	-16.578	52.373	0.504	1.00	37.29	CDK1
ATOM	1017	CG	PRO	194	-16.675	52.142	-0.964	1.00	38.67	CDK1
ATOM	1018	C	PRO	194	-15.083	51.420	2.340	1.00	44.63	CDK1
ATOM	1019	O	PRO	194	-14.517	52.103	3.206	1.00	48.14	CDK1
ATOM	1020	N	SER	195	-15.632	50.241	2.619	1.00	40.34	CDK1
ATOM	1021	CA	SER	195	-15.639	49.718	3.982	1.00	35.21	CDK1
ATOM	1022	CB	SER	195	-16.545	48.495	4.060	1.00	26.17	CDK1

ATOM	1023	OG	SER	195	-15.878	47.379	3.510	1.00	27.32	CDK1
ATOM	1024	C	SER	195	-14.278	49.369	4.580	1.00	36.09	CDK1
ATOM	1025	O	SER	195	-14.178	49.166	5.790	1.00	39.00	CDK1
ATOM	1026	N	ASN	196	-13.233	49.269	3.762	1.00	36.41	CDK1
ATOM	1027	CA	ASN	196	-11.907	48.950	4.302	1.00	26.38	CDK1
ATOM	1028	CB	ASN	196	-11.280	47.755	3.566	1.00	30.51	CDK1
ATOM	1029	CG	ASN	196	-12.033	46.441	3.830	1.00	39.46	CDK1
ATOM	1030	OD1	ASN	196	-12.965	46.413	4.633	1.00	45.75	CDK1
ATOM	1031	ND2	ASN	196	-11.631	45.356	3.159	1.00	28.32	CDK1
ATOM	1032	C	ASN	196	-10.993	50.168	4.252	1.00	26.73	CDK1
ATOM	1033	O	ASN	196	-9.777	50.047	4.221	1.00	26.84	CDK1
ATOM	1034	N	ILE	197	-11.599	51.350	4.224	1.00	33.41	CDK1
ATOM	1035	CA	ILE	197	-10.866	52.616	4.238	1.00	34.28	CDK1
ATOM	1036	CB	ILE	197	-11.162	53.496	2.988	1.00	31.76	CDK1
ATOM	1037	CG2	ILE	197	-10.331	54.767	3.033	1.00	27.11	CDK1
ATOM	1038	CG1	ILE	197	-10.866	52.712	1.703	1.00	36.65	CDK1
ATOM	1039	CD1	ILE	197	-11.138	53.490	0.422	1.00	32.46	CDK1
ATOM	1040	C	ILE	197	-11.434	53.306	5.484	1.00	37.59	CDK1
ATOM	1041	O	ILE	197	-12.587	53.749	5.497	1.00	35.03	CDK1
ATOM	1042	N	LEU	198	-10.632	53.381	6.535	1.00	36.49	CDK1
ATOM	1043	CA	LEU	198	-11.098	53.980	7.776	1.00	41.38	CDK1
ATOM	1044	CB	LEU	198	-10.584	53.147	8.941	1.00	32.98	CDK1
ATOM	1045	CG	LEU	198	-11.446	51.962	9.352	1.00	37.33	CDK1
ATOM	1046	CD1	LEU	198	-12.228	51.451	8.187	1.00	33.52	CDK1
ATOM	1047	CD2	LEU	198	-10.565	50.879	9.924	1.00	38.84	CDK1
ATOM	1048	C	LEU	198	-10.696	55.441	7.965	1.00	44.12	CDK1
ATOM	1049	O	LEU	198	-9.576	55.839	7.642	1.00	47.34	CDK1
ATOM	1050	N	VAL	199	-11.624	56.248	8.463	1.00	43.02	CDK1
ATOM	1051	CA	VAL	199	-11.319	57.652	8.722	1.00	48.28	CDK1
ATOM	1052	CB	VAL	199	-12.232	58.594	7.895	1.00	46.24	CDK1
ATOM	1053	CG1	VAL	199	-11.841	58.528	6.432	1.00	49.27	CDK1
ATOM	1054	CG2	VAL	199	-13.687	58.214	8.075	1.00	49.75	CDK1
ATOM	1055	C	VAL	199	-11.459	57.977	10.229	1.00	49.12	CDK1
ATOM	1056	O	VAL	199	-11.860	57.123	11.023	1.00	45.64	CDK1
ATOM	1057	N	ASN	200	-11.092	59.197	10.622	1.00	49.47	CDK1
ATOM	1058	CA	ASN	200	-11.198	59.608	12.018	1.00	47.10	CDK1
ATOM	1059	CB	ASN	200	-10.042	59.015	12.844	1.00	32.98	CDK1
ATOM	1060	CG	ASN	200	-8.728	59.766	12.680	1.00	39.34	CDK1
ATOM	1061	OD1	ASN	200	-7.672	59.265	13.080	1.00	40.04	CDK1
ATOM	1062	ND2	ASN	200	-8.777	60.959	12.110	1.00	33.26	CDK1
ATOM	1063	C	ASN	200	-11.307	61.123	12.200	1.00	52.62	CDK1
ATOM	1064	O	ASN	200	-10.941	61.900	11.318	1.00	47.44	CDK1
ATOM	1065	N	SER	201	-11.833	61.530	13.351	1.00	60.21	CDK1

ATOM	1066	CA	SER	201	-12.042	62.943	13.672	1.00	63.99	CDK1
ATOM	1067	CB	SER	201	-12.475	63.069	15.124	1.00	59.89	CDK1
ATOM	1068	OG	SER	201	-11.588	62.334	15.942	1.00	64.14	CDK1
ATOM	1069	C	SER	201	-10.816	63.816	13.442	1.00	65.64	CDK1
ATOM	1070	O	SER	201	-10.920	65.029	13.290	1.00	66.70	CDK1
ATOM	1071	N	ARG	202	-9.652	63.192	13.421	1.00	67.54	CDK1
ATOM	1072	CA	ARG	202	-8.412	63.917	13.224	1.00	66.63	CDK1
ATOM	1073	CB	ARG	202	-7.271	63.114	13.830	1.00	69.61	CDK1
ATOM	1074	CG	ARG	202	-7.751	62.093	14.855	1.00	78.51	CDK1
ATOM	1075	CD	ARG	202	-6.746	61.933	15.966	1.00	85.70	CDK1
ATOM	1076	NE	ARG	202	-5.389	61.822	15.441	1.00	92.72	CDK1
ATOM	1077	CZ	ARG	202	-4.712	60.681	15.365	1.00	98.60	CDK1
ATOM	1078	NH1	ARG	202	-5.267	59.546	15.782	1.00	100.00	CDK1
ATOM	1079	NH2	ARG	202	-3.479	60.673	14.867	1.00	100.00	CDK1
ATOM	1080	C	ARG	202	-8.135	64.199	11.756	1.00	66.96	CDK1
ATOM	1081	O	ARG	202	-7.156	64.860	11.427	1.00	71.35	CDK1
ATOM	1082	N	GLY	203	-8.995	63.705	10.871	1.00	64.87	CDK1
ATOM	1083	CA	GLY	203	-8.797	63.936	9.448	1.00	62.43	CDK1
ATOM	1084	C	GLY	203	-7.940	62.881	8.770	1.00	57.70	CDK1
ATOM	1085	O	GLY	203	-7.580	63.007	7.598	1.00	51.17	CDK1
ATOM	1086	N	GLU	204	-7.623	61.832	9.521	1.00	57.83	CDK1
ATOM	1087	CA	GLU	204	-6.808	60.737	9.018	1.00	57.63	CDK1
ATOM	1088	CB	GLU	204	-6.131	60.021	10.193	1.00	59.21	CDK1
ATOM	1089	CG	GLU	204	-4.783	60.615	10.603	1.00	61.87	CDK1
ATOM	1090	CD	GLU	204	-4.190	59.941	11.831	1.00	65.24	CDK1
ATOM	1091	OE1	GLU	204	-4.955	59.649	12.773	1.00	65.94	CDK1
ATOM	1092	OE2	GLU	204	-2.962	59.699	11.857	1.00	67.59	CDK1
ATOM	1093	C	GLU	204	-7.626	59.741	8.172	1.00	55.60	CDK1
ATOM	1094	O	GLU	204	-8.811	59.504	8.415	1.00	52.71	CDK1
ATOM	1095	N	ILE	205	-6.970	59.169	7.170	1.00	52.72	CDK1
ATOM	1096	CA	ILE	205	-7.604	58.219	6.266	1.00	46.58	CDK1
ATOM	1097	CB	ILE	205	-7.807	58.850	4.885	1.00	44.45	CDK1
ATOM	1098	CG2	ILE	205	-8.546	57.886	3.989	1.00	47.47	CDK1
ATOM	1099	CG1	ILE	205	-8.561	60.180	5.030	1.00	43.77	CDK1
ATOM	1100	CD1	ILE	205	-8.886	60.873	3.704	1.00	46.52	CDK1
ATOM	1101	C	ILE	205	-6.653	57.057	6.141	1.00	42.70	CDK1
ATOM	1102	O	ILE	205	-5.546	57.227	5.645	1.00	41.44	CDK1
ATOM	1103	N	LYS	206	-7.075	55.877	6.587	1.00	40.82	CDK1
ATOM	1104	CA	LYS	206	-6.202	54.715	6.544	1.00	33.80	CDK1
ATOM	1105	CB	LYS	206	-5.694	54.398	7.951	1.00	43.43	CDK1
ATOM	1106	CG	LYS	206	-5.341	55.618	8.778	1.00	45.41	CDK1
ATOM	1107	CD	LYS	206	-4.585	55.216	10.053	1.00	51.29	CDK1
ATOM	1108	CE	LYS	206	-3.855	56.410	10.670	1.00	47.41	CDK1

ATOM	1109	NZ	LYS	206	-3.650	56.270	12.136	1.00	47.69	CDK1
ATOM	1110	C	LYS	206	-6.840	53.475	5.965	1.00	32.65	CDK1
ATOM	1111	O	LYS	206	-8.059	53.366	5.875	1.00	34.25	CDK1
ATOM	1112	N	LEU	207	-5.990	52.520	5.616	1.00	31.60	CDK1
ATOM	1113	CA	LEU	207	-6.419	51.258	5.028	1.00	33.33	CDK1
ATOM	1114	CB	LEU	207	-5.522	50.882	3.833	1.00	34.61	CDK1
ATOM	1115	CG	LEU	207	-5.726	51.277	2.374	1.00	30.82	CDK1
ATOM	1116	CD1	LEU	207	-6.665	52.420	2.211	1.00	34.23	CDK1
ATOM	1117	CD2	LEU	207	-4.397	51.639	1.831	1.00	24.90	CDK1
ATOM	1118	C	LEU	207	-6.293	50.127	6.021	1.00	33.20	CDK1
ATOM	1119	O	LEU	207	-5.303	50.041	6.748	1.00	34.47	CDK1
ATOM	1120	N	CYS	208	-7.271	49.234	6.016	1.00	27.95	CDK1
ATOM	1121	CA	CYS	208	-7.223	48.058	6.871	1.00	31.63	CDK1
ATOM	1122	CB	CYS	208	-8.280	48.130	7.960	1.00	29.75	CDK1
ATOM	1123	SG	CYS	208	-9.930	48.318	7.270	1.00	36.61	CDK1
ATOM	1124	C	CYS	208	-7.543	46.856	6.002	1.00	36.74	CDK1
ATOM	1125	O	CYS	208	-7.766	46.977	4.797	1.00	33.98	CDK1
ATOM	1126	N	ASP	209	-7.568	45.694	6.635	1.00	39.00	CDK1
ATOM	1127	CA	ASP	209	-7.921	44.458	5.972	1.00	40.54	CDK1
ATOM	1128	CB	ASP	209	-9.421	44.483	5.653	1.00	41.88	CDK1
ATOM	1129	CG	ASP	209	-10.285	44.454	6.897	1.00	45.90	CDK1
ATOM	1130	OD1	ASP	209	-11.483	44.762	6.792	1.00	43.66	CDK1
ATOM	1131	OD2	ASP	209	-9.772	44.122	7.983	1.00	49.77	CDK1
ATOM	1132	C	ASP	209	-7.144	44.059	4.713	1.00	42.06	CDK1
ATOM	1133	O	ASP	209	-7.747	43.562	3.760	1.00	41.33	CDK1
ATOM	1134	N	PHE	210	-5.829	44.262	4.693	1.00	37.85	CDK1
ATOM	1135	CA	PHE	210	-5.057	43.850	3.535	1.00	42.09	CDK1
ATOM	1136	CB	PHE	210	-3.883	44.786	3.266	1.00	40.96	CDK1
ATOM	1137	CG	PHE	210	-3.238	45.328	4.491	1.00	36.21	CDK1
ATOM	1138	CD1	PHE	210	-3.708	46.502	5.070	1.00	41.00	CDK1
ATOM	1139	CD2	PHE	210	-2.106	44.720	5.012	1.00	30.89	CDK1
ATOM	1140	CE1	PHE	210	-3.054	47.070	6.148	1.00	37.05	CDK1
ATOM	1141	CE2	PHE	210	-1.441	45.272	6.084	1.00	32.91	CDK1
ATOM	1142	CZ	PHE	210	-1.917	46.455	6.654	1.00	37.53	CDK1
ATOM	1143	C	PHE	210	-4.570	42.431	3.762	1.00	43.82	CDK1
ATOM	1144	O	PHE	210	-4.702	41.915	4.858	1.00	43.37	CDK1
ATOM	1145	N	GLY	211	-4.005	41.808	2.730	1.00	42.75	CDK1
ATOM	1146	CA	GLY	211	-3.569	40.427	2.841	1.00	40.45	CDK1
ATOM	1147	C	GLY	211	-2.141	40.173	3.261	1.00	46.95	CDK1
ATOM	1148	O	GLY	211	-1.278	39.936	2.408	1.00	46.58	CDK1
ATOM	1149	N	VAL	212	-1.892	40.194	4.573	1.00	41.91	CDK1
ATOM	1150	CA	VAL	212	-0.554	39.957	5.108	1.00	39.14	CDK1
ATOM	1151	CB	VAL	212	-0.332	40.664	6.484	1.00	38.71	CDK1

ATOM	1152	CG1	VAL	212	-0.055	42.140	6.276	1.00 43.39	CDK1
ATOM	1153	CG2	VAL	212	-1.558	40.477	7.386	1.00 31.35	CDK1
ATOM	1154	C	VAL	212	-0.287	38.471	5.313	1.00 41.55	CDK1
ATOM	1155	O	VAL	212	0.866	38.049	5.393	1.00 46.32	CDK1
ATOM	1156	N	SER	213	-1.346	37.676	5.399	1.00 39.36	CDK1
ATOM	1157	CA	SER	213	-1.168	36.252	5.630	1.00 40.11	CDK1
ATOM	1158	CB	SER	213	-1.820	35.854	6.967	1.00 45.77	CDK1
ATOM	1159	OG	SER	213	-2.261	34.499	6.998	1.00 37.98	CDK1
ATOM	1160	C	SER	213	-1.699	35.370	4.511	1.00 40.97	CDK1
ATOM	1161	O	SER	213	-2.906	35.317	4.243	1.00 34.74	CDK1
ATOM	1162	N	GLY	214	-0.784	34.668	3.859	1.00 41.74	CDK1
ATOM	1163	CA	GLY	214	-1.195	33.777	2.798	1.00 45.99	CDK1
ATOM	1164	C	GLY	214	-2.156	32.750	3.356	1.00 45.47	CDK1
ATOM	1165	O	GLY	214	-3.179	32.424	2.741	1.00 43.51	CDK1
ATOM	1166	N	GLN	215	-1.822	32.244	4.541	1.00 50.63	CDK1
ATOM	1167	CA	GLN	215	-2.641	31.238	5.208	1.00 48.48	CDK1
ATOM	1168	CB	GLN	215	-1.958	30.762	6.493	1.00 53.76	CDK1
ATOM	1169	CG	GLN	215	-1.793	29.260	6.586	1.00 55.51	CDK1
ATOM	1170	CD	GLN	215	-2.927	28.522	5.916	1.00 60.04	CDK1
ATOM	1171	OE1	GLN	215	-4.095	28.873	6.086	1.00 62.33	CDK1
ATOM	1172	NE2	GLN	215	-2.592	27.497	5.145	1.00 57.24	CDK1
ATOM	1173	C	GLN	215	-4.021	31.799	5.520	1.00 47.39	CDK1
ATOM	1174	O	GLN	215	-5.015	31.077	5.456	1.00 47.96	CDK1
ATOM	1175	N	LEU	216	-4.091	33.086	5.859	1.00 45.09	CDK1
ATOM	1176	CA	LEU	216	-5.387	33.683	6.139	1.00 45.86	CDK1
ATOM	1177	CB	LEU	216	-5.243	35.081	6.752	1.00 45.00	CDK1
ATOM	1178	CG	LEU	216	-6.507	35.520	7.499	1.00 46.21	CDK1
ATOM	1179	CD1	LEU	216	-7.117	34.309	8.191	1.00 35.59	CDK1
ATOM	1180	CD2	LEU	216	-6.181	36.595	8.510	1.00 44.27	CDK1
ATOM	1181	C	LEU	216	-6.153	33.749	4.821	1.00 48.22	CDK1
ATOM	1182	O	LEU	216	-7.286	33.266	4.738	1.00 46.36	CDK1
ATOM	1183	N	ILE	217	-5.520	34.322	3.790	1.00 48.35	CDK1
ATOM	1184	CA	ILE	217	-6.128	34.419	2.458	1.00 49.65	CDK1
ATOM	1185	CB	ILE	217	-5.079	34.792	1.371	1.00 47.77	CDK1
ATOM	1186	CG2	ILE	217	-5.667	34.589	-0.023	1.00 47.48	CDK1
ATOM	1187	CG1	ILE	217	-4.683	36.258	1.476	1.00 40.61	CDK1
ATOM	1188	CD1	ILE	217	-3.259	36.534	1.009	1.00 41.04	CDK1
ATOM	1189	C	ILE	217	-6.713	33.040	2.100	1.00 52.30	CDK1
ATOM	1190	O	ILE	217	-7.887	32.912	1.727	1.00 48.47	CDK1
ATOM	1191	N	ASP	218	-5.878	32.013	2.222	1.00 54.85	CDK1
ATOM	1192	CA	ASP	218	-6.299	30.656	1.920	1.00 61.04	CDK1
ATOM	1193	CB	ASP	218	-5.187	29.665	2.272	1.00 69.47	CDK1
ATOM	1194	CG	ASP	218	-4.168	29.513	1.156	1.00 79.30	CDK1

ATOM	1195	OD1	ASP	218	-4.111	30.403	0.276	1.00	83.30	CDK1
ATOM	1196	OD2	ASP	218	-3.422	28.505	1.156	1.00	84.20	CDK1
ATOM	1197	C	ASP	218	-7.555	30.311	2.701	1.00	61.92	CDK1
ATOM	1198	O	ASP	218	-8.628	30.156	2.122	1.00	60.20	CDK1
ATOM	1199	N	SER	219	-7.422	30.213	4.020	1.00	61.64	CDK1
ATOM	1200	CA	SER	219	-8.547	29.861	4.872	1.00	62.74	CDK1
ATOM	1201	CB	SER	219	-8.109	29.829	6.330	1.00	60.68	CDK1
ATOM	1202	OG	SER	219	-7.046	28.916	6.484	1.00	62.79	CDK1
ATOM	1203	C	SER	219	-9.764	30.750	4.725	1.00	64.64	CDK1
ATOM	1204	O	SER	219	-10.754	30.560	5.418	1.00	67.75	CDK1
ATOM	1205	N	MET	220	-9.704	31.731	3.841	1.00	69.53	CDK1
ATOM	1206	CA	MET	220	-10.864	32.584	3.635	1.00	76.98	CDK1
ATOM	1207	CB	MET	220	-10.487	34.064	3.787	1.00	77.28	CDK1
ATOM	1208	CG	MET	220	-9.612	34.380	5.000	1.00	79.21	CDK1
ATOM	1209	SD	MET	220	-10.371	35.434	6.268	1.00	78.08	CDK1
ATOM	1210	CE	MET	220	-11.606	34.292	6.924	1.00	70.02	CDK1
ATOM	1211	C	MET	220	-11.410	32.305	2.233	1.00	80.06	CDK1
ATOM	1212	O	MET	220	-11.685	33.223	1.460	1.00	83.43	CDK1
ATOM	1213	N	ALA	221	-11.561	31.021	1.920	1.00	83.08	CDK1
ATOM	1214	CA	ALA	221	-12.066	30.578	0.620	1.00	82.29	CDK1
ATOM	1215	CB	ALA	221	-11.884	29.068	0.484	1.00	80.44	CDK1
ATOM	1216	C	ALA	221	-13.534	30.941	0.401	1.00	82.23	CDK1
ATOM	1217	O	ALA	221	-13.893	31.501	-0.638	1.00	78.47	CDK1
ATOM	1218	N	ASN	222	-14.373	30.623	1.387	1.00	83.70	CDK1
ATOM	1219	CA	ASN	222	-15.814	30.886	1.320	1.00	83.23	CDK1
ATOM	1220	CB	ASN	222	-16.581	29.749	2.015	1.00	82.64	CDK1
ATOM	1221	CG	ASN	222	-16.028	28.361	1.673	1.00	85.09	CDK1
ATOM	1222	OD1	ASN	222	-14.841	28.200	1.371	1.00	81.92	CDK1
ATOM	1223	ND2	ASN	222	-16.897	27.350	1.723	1.00	86.26	CDK1
ATOM	1224	C	ASN	222	-16.240	32.239	1.916	1.00	80.42	CDK1
ATOM	1225	O	ASN	222	-17.063	32.923	1.274	1.00	76.53	CDK1
ATOM	1226	OT	ASN	222	-15.757	32.603	3.014	1.00	80.92	CDK1
ATOM	1227	CB	VAL	225	-17.531	40.172	-1.163	1.00	96.71	CDK2
ATOM	1228	CG1	VAL	225	-18.443	41.304	-1.649	1.00	98.94	CDK2
ATOM	1229	CG2	VAL	225	-16.609	40.684	-0.068	1.00	94.24	CDK2
ATOM	1230	C	VAL	225	-19.738	38.919	-1.288	1.00	94.14	CDK2
ATOM	1231	O	VAL	225	-19.970	38.104	-2.180	1.00	95.78	CDK2
ATOM	1232	N	VAL	225	-17.665	37.669	-0.895	1.00	96.27	CDK2
ATOM	1233	CA	VAL	225	-18.365	38.961	-0.623	1.00	95.65	CDK2
ATOM	1234	N	GLY	226	-20.648	39.779	-0.839	1.00	92.50	CDK2
ATOM	1235	CA	GLY	226	-21.982	39.806	-1.413	1.00	90.19	CDK2
ATOM	1236	C	GLY	226	-21.983	40.184	-2.884	1.00	88.16	CDK2
ATOM	1237	O	GLY	226	-20.925	40.198	-3.521	1.00	87.24	CDK2

ATOM	1238	N	THR	227	-23.171	40.476	-3.421	1.00	84.61	CDK2
ATOM	1239	CA	THR	227	-23.331	40.875	-4.820	1.00	77.94	CDK2
ATOM	1240	CB	THR	227	-24.729	41.481	-5.076	1.00	79.05	CDK2
ATOM	1241	OG1	THR	227	-25.597	41.148	-3.988	1.00	72.89	CDK2
ATOM	1242	CG2	THR	227	-25.319	40.958	-6.397	1.00	77.02	CDK2
ATOM	1243	C	THR	227	-22.284	41.932	-5.184	1.00	76.19	CDK2
ATOM	1244	O	THR	227	-21.242	41.615	-5.760	1.00	78.54	CDK2
ATOM	1245	N	ARG	228	-22.567	43.187	-4.849	1.00	67.16	CDK2
ATOM	1246	CA	ARG	228	-21.644	44.277	-5.131	1.00	63.25	CDK2
ATOM	1247	CB	ARG	228	-21.942	45.441	-4.183	1.00	62.74	CDK2
ATOM	1248	CG	ARG	228	-23.410	45.855	-4.194	1.00	69.29	CDK2
ATOM	1249	CD	ARG	228	-23.916	46.215	-2.806	1.00	75.28	CDK2
ATOM	1250	NE	ARG	228	-24.025	47.661	-2.616	1.00	76.75	CDK2
ATOM	1251	CZ	ARG	228	-22.995	48.459	-2.337	1.00	76.48	CDK2
ATOM	1252	NH1	ARG	228	-21.774	47.952	-2.215	1.00	77.38	CDK2
ATOM	1253	NH2	ARG	228	-23.184	49.765	-2.179	1.00	71.79	CDK2
ATOM	1254	C	ARG	228	-20.173	43.836	-5.009	1.00	60.44	CDK2
ATOM	1255	O	ARG	228	-19.658	43.643	-3.904	1.00	66.04	CDK2
ATOM	1256	N	SER	229	-19.511	43.664	-6.152	1.00	50.91	CDK2
ATOM	1257	CA	SER	229	-18.107	43.252	-6.192	1.00	44.26	CDK2
ATOM	1258	CB	SER	229	-17.912	42.114	-7.196	1.00	39.65	CDK2
ATOM	1259	OG	SER	229	-16.635	41.524	-7.045	1.00	40.81	CDK2
ATOM	1260	C	SER	229	-17.181	44.407	-6.567	1.00	40.73	CDK2
ATOM	1261	O	SER	229	-17.570	45.315	-7.288	1.00	41.83	CDK2
ATOM	1262	N	TYR	230	-15.957	44.381	-6.055	1.00	42.20	CDK2
ATOM	1263	CA	TYR	230	-14.985	45.418	-6.363	1.00	34.83	CDK2
ATOM	1264	CB	TYR	230	-14.549	46.178	-5.105	1.00	32.07	CDK2
ATOM	1265	CG	TYR	230	-15.656	46.987	-4.473	1.00	30.29	CDK2
ATOM	1266	CD1	TYR	230	-15.830	48.327	-4.777	1.00	30.04	CDK2
ATOM	1267	CE1	TYR	230	-16.906	49.050	-4.253	1.00	35.06	CDK2
ATOM	1268	CD2	TYR	230	-16.576	46.383	-3.617	1.00	33.27	CDK2
ATOM	1269	CE2	TYR	230	-17.645	47.089	-3.093	1.00	26.32	CDK2
ATOM	1270	CZ	TYR	230	-17.810	48.415	-3.417	1.00	33.72	CDK2
ATOM	1271	OH	TYR	230	-18.913	49.078	-2.943	1.00	36.86	CDK2
ATOM	1272	C	TYR	230	-13.806	44.707	-6.982	1.00	33.07	CDK2
ATOM	1273	O	TYR	230	-12.737	45.295	-7.173	1.00	32.91	CDK2
ATOM	1274	N	MET	231	-14.012	43.426	-7.282	1.00	27.75	CDK2
ATOM	1275	CA	MET	231	-12.982	42.618	-7.919	1.00	34.74	CDK2
ATOM	1276	CB	MET	231	-13.402	41.163	-7.982	1.00	41.48	CDK2
ATOM	1277	CG	MET	231	-13.857	40.587	-6.693	1.00	41.98	CDK2
ATOM	1278	SD	MET	231	-12.978	39.068	-6.468	1.00	51.04	CDK2
ATOM	1279	CE	MET	231	-14.039	38.292	-5.238	1.00	57.85	CDK2
ATOM	1280	C	MET	231	-12.729	43.087	-9.364	1.00	37.37	CDK2

ATOM	1281	O	MET	231	-13.653	43.455	-10.093	1.00	29.01	CDK2
ATOM	1282	N	SER	232	-11.468	43.054	-9.769	1.00	35.06	CDK2
ATOM	1283	CA	SER	232	-11.110	43.459	-11.108	1.00	37.18	CDK2
ATOM	1284	CB	SER	232	-9.591	43.659	-11.220	1.00	29.03	CDK2
ATOM	1285	OG	SER	232	-8.933	42.415	-11.374	1.00	28.99	CDK2
ATOM	1286	C	SER	232	-11.572	42.370	-12.075	1.00	39.52	CDK2
ATOM	1287	O	SER	232	-11.758	41.197	-11.694	1.00	37.59	CDK2
ATOM	1288	N	PRO	233	-11.783	42.750	-13.344	1.00	39.25	CDK2
ATOM	1289	CD	PRO	233	-11.643	44.113	-13.883	1.00	39.41	CDK2
ATOM	1290	CA	PRO	233	-12.222	41.797	-14.367	1.00	35.72	CDK2
ATOM	1291	CB	PRO	233	-12.236	42.619	-15.646	1.00	39.66	CDK2
ATOM	1292	CG	PRO	233	-12.382	44.029	-15.184	1.00	40.71	CDK2
ATOM	1293	C	PRO	233	-11.271	40.616	-14.455	1.00	32.71	CDK2
ATOM	1294	O	PRO	233	-11.714	39.466	-14.567	1.00	32.61	CDK2
ATOM	1295	N	GLU	234	-9.969	40.889	-14.382	1.00	25.80	CDK2
ATOM	1296	CA	GLU	234	-8.997	39.796	-14.460	1.00	31.29	CDK2
ATOM	1297	CB	GLU	234	-7.548	40.331	-14.615	1.00	27.93	CDK2
ATOM	1298	CG	GLU	234	-6.941	41.038	-13.420	1.00	35.25	CDK2
ATOM	1299	CD	GLU	234	-7.122	42.543	-13.491	1.00	46.04	CDK2
ATOM	1300	OE1	GLU	234	-6.343	43.244	-12.792	1.00	34.59	CDK2
ATOM	1301	OE2	GLU	234	-8.042	43.011	-14.235	1.00	34.13	CDK2
ATOM	1302	C	GLU	234	-9.126	38.866	-13.252	1.00	36.15	CDK2
ATOM	1303	O	GLU	234	-9.230	37.642	-13.415	1.00	36.00	CDK2
ATOM	1304	N	ARG	235	-9.152	39.443	-12.046	1.00	36.25	CDK2
ATOM	1305	CA	ARG	235	-9.308	38.631	-10.842	1.00	30.67	CDK2
ATOM	1306	CB	ARG	235	-9.357	39.498	-9.589	1.00	33.14	CDK2
ATOM	1307	CG	ARG	235	-8.916	38.751	-8.347	1.00	38.41	CDK2
ATOM	1308	CD	ARG	235	-9.155	39.546	-7.078	1.00	35.72	CDK2
ATOM	1309	NE	ARG	235	-9.403	38.641	-5.970	1.00	49.08	CDK2
ATOM	1310	CZ	ARG	235	-9.156	38.906	-4.692	1.00	43.29	CDK2
ATOM	1311	NH1	ARG	235	-8.643	40.073	-4.320	1.00	36.78	CDK2
ATOM	1312	NH2	ARG	235	-9.407	37.972	-3.796	1.00	35.72	CDK2
ATOM	1313	C	ARG	235	-10.588	37.825	-10.946	1.00	26.85	CDK2
ATOM	1314	O	ARG	235	-10.589	36.640	-10.646	1.00	30.69	CDK2
ATOM	1315	N	LEU	236	-11.674	38.459	-11.388	1.00	22.65	CDK2
ATOM	1316	CA	LEU	236	-12.947	37.759	-11.539	1.00	29.34	CDK2
ATOM	1317	CB	LEU	236	-14.015	38.722	-12.040	1.00	25.84	CDK2
ATOM	1318	CG	LEU	236	-14.711	39.705	-11.106	1.00	37.33	CDK2
ATOM	1319	CD1	LEU	236	-15.989	40.164	-11.777	1.00	28.71	CDK2
ATOM	1320	CD2	LEU	236	-15.032	39.051	-9.761	1.00	35.07	CDK2
ATOM	1321	C	LEU	236	-12.876	36.568	-12.517	1.00	36.60	CDK2
ATOM	1322	O	LEU	236	-13.612	35.591	-12.371	1.00	39.06	CDK2
ATOM	1323	N	GLN	237	-11.983	36.637	-13.505	1.00	38.27	CDK2

ATOM	1324	CA	GLN	237	-11.894	35.572	-14.500	1.00	40.29	CDK2
ATOM	1325	CB	GLN	237	-11.702	36.198	-15.895	1.00	41.52	CDK2
ATOM	1326	CG	GLN	237	-13.006	36.799	-16.460	1.00	45.94	CDK2
ATOM	1327	CD	GLN	237	-12.798	37.893	-17.528	1.00	55.13	CDK2
ATOM	1328	OE1	GLN	237	-11.707	38.449	-17.673	1.00	48.77	CDK2
ATOM	1329	NE2	GLN	237	-13.864	38.204	-18.268	1.00	55.35	CDK2
ATOM	1330	C	GLN	237	-10.866	34.457	-14.260	1.00	40.06	CDK2
ATOM	1331	O	GLN	237	-11.048	33.328	-14.725	1.00	42.61	CDK2
ATOM	1332	N	GLY	238	-9.792	34.738	-13.537	1.00	36.28	CDK2
ATOM	1333	CA	GLY	238	-8.836	33.671	-13.308	1.00	36.18	CDK2
ATOM	1334	C	GLY	238	-7.776	34.012	-12.289	1.00	41.42	CDK2
ATOM	1335	O	GLY	238	-7.970	34.867	-11.439	1.00	42.04	CDK2
ATOM	1336	N	THR	239	-6.647	33.329	-12.402	1.00	47.91	CDK2
ATOM	1337	CA	THR	239	-5.496	33.502	-11.522	1.00	51.06	CDK2
ATOM	1338	CB	THR	239	-4.719	32.171	-11.392	1.00	54.87	CDK2
ATOM	1339	OG1	THR	239	-3.981	31.944	-12.604	1.00	59.65	CDK2
ATOM	1340	CG2	THR	239	-5.672	30.992	-11.181	1.00	52.61	CDK2
ATOM	1341	C	THR	239	-4.501	34.540	-12.066	1.00	52.06	CDK2
ATOM	1342	O	THR	239	-3.462	34.796	-11.451	1.00	52.89	CDK2
ATOM	1343	N	HIS	240	-4.795	35.125	-13.220	1.00	52.16	CDK2
ATOM	1344	CA	HIS	240	-3.861	36.085	-13.792	1.00	52.77	CDK2
ATOM	1345	CB	HIS	240	-3.808	35.940	-15.314	1.00	54.03	CDK2
ATOM	1346	CG	HIS	240	-3.257	34.623	-15.769	1.00	57.16	CDK2
ATOM	1347	CD2	HIS	240	-1.988	34.154	-15.810	1.00	57.93	CDK2
ATOM	1348	ND1	HIS	240	-4.058	33.595	-16.220	1.00	59.40	CDK2
ATOM	1349	CE1	HIS	240	-3.308	32.550	-16.518	1.00	56.19	CDK2
ATOM	1350	NE2	HIS	240	-2.047	32.863	-16.277	1.00	59.84	CDK2
ATOM	1351	C	HIS	240	-4.149	37.522	-13.408	1.00	51.27	CDK2
ATOM	1352	O	HIS	240	-4.684	38.315	-14.198	1.00	52.88	CDK2
ATOM	1353	N	TYR	241	-3.788	37.844	-12.174	1.00	45.79	CDK2
ATOM	1354	CA	TYR	241	-3.956	39.180	-11.649	1.00	43.36	CDK2
ATOM	1355	CB	TYR	241	-5.353	39.359	-11.065	1.00	47.66	CDK2
ATOM	1356	CG	TYR	241	-5.532	38.616	-9.771	1.00	54.30	CDK2
ATOM	1357	CD1	TYR	241	-5.471	39.283	-8.544	1.00	56.86	CDK2
ATOM	1358	CE1	TYR	241	-5.579	38.592	-7.342	1.00	51.46	CDK2
ATOM	1359	CD2	TYR	241	-5.711	37.236	-9.766	1.00	54.60	CDK2
ATOM	1360	CE2	TYR	241	-5.821	36.536	-8.578	1.00	58.01	CDK2
ATOM	1361	CZ	TYR	241	-5.751	37.219	-7.370	1.00	56.44	CDK2
ATOM	1362	OH	TYR	241	-5.832	36.516	-6.201	1.00	57.07	CDK2
ATOM	1363	C	TYR	241	-2.913	39.351	-10.559	1.00	42.95	CDK2
ATOM	1364	O	TYR	241	-2.317	38.368	-10.097	1.00	38.50	CDK2
ATOM	1365	N	SER	242	-2.691	40.603	-10.164	1.00	37.42	CDK2
ATOM	1366	CA	SER	242	-1.741	40.939	-9.119	1.00	29.57	CDK2

ATOM	1367	CB	SER	242	-0.316	40.863	-9.666	1.00	34.82	CDK2
ATOM	1368	OG	SER	242	0.619	41.387	-8.737	1.00	44.90	CDK2
ATOM	1369	C	SER	242	-2.043	42.336	-8.569	1.00	25.30	CDK2
ATOM	1370	O	SER	242	-3.211	42.722	-8.466	1.00	26.18	CDK2
ATOM	1371	N	VAL	243	-1.005	43.107	-8.251	1.00	25.51	CDK2
ATOM	1372	CA	VAL	243	-1.191	44.432	-7.670	1.00	32.16	CDK2
ATOM	1373	CB	VAL	243	0.156	45.050	-7.326	1.00	40.33	CDK2
ATOM	1374	CG1	VAL	243	0.943	44.086	-6.451	1.00	39.31	CDK2
ATOM	1375	CG2	VAL	243	0.909	45.372	-8.602	1.00	40.74	CDK2
ATOM	1376	C	VAL	243	-2.002	45.446	-8.468	1.00	38.53	CDK2
ATOM	1377	O	VAL	243	-2.588	46.376	-7.886	1.00	38.34	CDK2
ATOM	1378	N	GLN	244	-2.027	45.288	-9.793	1.00	36.78	CDK2
ATOM	1379	CA	GLN	244	-2.792	46.186	-10.650	1.00	30.13	CDK2
ATOM	1380	CB	GLN	244	-2.592	45.807	-12.128	1.00	41.56	CDK2
ATOM	1381	CG	GLN	244	-1.484	46.572	-12.864	1.00	36.91	CDK2
ATOM	1382	CD	GLN	244	-1.439	48.041	-12.514	1.00	39.13	CDK2
ATOM	1383	OE1	GLN	244	-0.749	48.437	-11.587	1.00	44.56	CDK2
ATOM	1384	NE2	GLN	244	-2.178	48.859	-13.259	1.00	44.07	CDK2
ATOM	1385	C	GLN	244	-4.268	46.065	-10.290	1.00	28.12	CDK2
ATOM	1386	O	GLN	244	-5.029	47.020	-10.409	1.00	36.39	CDK2
ATOM	1387	N	SER	245	-4.676	44.870	-9.873	1.00	29.37	CDK2
ATOM	1388	CA	SER	245	-6.060	44.614	-9.477	1.00	28.17	CDK2
ATOM	1389	CB	SER	245	-6.189	43.181	-8.997	1.00	26.36	CDK2
ATOM	1390	OG	SER	245	-7.547	42.804	-9.000	1.00	41.30	CDK2
ATOM	1391	C	SER	245	-6.586	45.575	-8.387	1.00	33.42	CDK2
ATOM	1392	O	SER	245	-7.793	45.860	-8.331	1.00	34.65	CDK2
ATOM	1393	N	ASP	246	-5.683	46.082	-7.538	1.00	31.38	CDK2
ATOM	1394	CA	ASP	246	-6.072	47.009	-6.483	1.00	36.15	CDK2
ATOM	1395	CB	ASP	246	-4.920	47.241	-5.483	1.00	40.03	CDK2
ATOM	1396	CG	ASP	246	-4.655	46.036	-4.556	1.00	39.89	CDK2
ATOM	1397	OD1	ASP	246	-3.480	45.863	-4.158	1.00	35.19	CDK2
ATOM	1398	OD2	ASP	246	-5.596	45.266	-4.228	1.00	36.20	CDK2
ATOM	1399	C	ASP	246	-6.481	48.352	-7.081	1.00	41.37	CDK2
ATOM	1400	O	ASP	246	-7.352	49.050	-6.528	1.00	41.85	CDK2
ATOM	1401	N	ILE	247	-5.857	48.719	-8.208	1.00	40.77	CDK2
ATOM	1402	CA	ILE	247	-6.153	49.994	-8.861	1.00	37.16	CDK2
ATOM	1403	CB	ILE	247	-5.234	50.268	-10.095	1.00	42.74	CDK2
ATOM	1404	CG2	ILE	247	-5.637	51.597	-10.777	1.00	36.99	CDK2
ATOM	1405	CG1	ILE	247	-3.779	50.367	-9.644	1.00	36.34	CDK2
ATOM	1406	CD1	ILE	247	-3.550	51.437	-8.603	1.00	40.80	CDK2
ATOM	1407	C	ILE	247	-7.592	50.045	-9.317	1.00	35.14	CDK2
ATOM	1408	O	ILE	247	-8.269	51.065	-9.132	1.00	33.24	CDK2
ATOM	1409	N	TRP	248	-8.060	48.948	-9.913	1.00	39.12	CDK2

ATOM	1410	CA	TRP	248	-9.444	48.867	-10.393	1.00	38.37	CDK2
ATOM	1411	CB	TRP	248	-9.706	47.486	-11.036	1.00	37.84	CDK2
ATOM	1412	CG	TRP	248	-11.170	47.203	-11.309	1.00	41.03	CDK2
ATOM	1413	CD2	TRP	248	-11.871	47.442	-12.533	1.00	47.69	CDK2
ATOM	1414	CE2	TRP	248	-13.233	47.124	-12.307	1.00	51.25	CDK2
ATOM	1415	CE3	TRP	248	-11.484	47.899	-13.802	1.00	45.71	CDK2
ATOM	1416	CD1	TRP	248	-12.108	46.751	-10.416	1.00	44.55	CDK2
ATOM	1417	NE1	TRP	248	-13.351	46.705	-11.008	1.00	44.17	CDK2
ATOM	1418	CZ2	TRP	248	-14.209	47.251	-13.310	1.00	54.89	CDK2
ATOM	1419	CZ3	TRP	248	-12.453	48.029	-14.793	1.00	48.74	CDK2
ATOM	1420	CH2	TRP	248	-13.799	47.707	-14.542	1.00	47.54	CDK2
ATOM	1421	C	TRP	248	-10.399	49.105	-9.203	1.00	40.74	CDK2
ATOM	1422	O	TRP	248	-11.292	49.982	-9.251	1.00	35.01	CDK2
ATOM	1423	N	SER	249	-10.188	48.339	-8.130	1.00	36.81	CDK2
ATOM	1424	CA	SER	249	-11.021	48.455	-6.921	1.00	34.72	CDK2
ATOM	1425	CB	SER	249	-10.475	47.567	-5.793	1.00	32.01	CDK2
ATOM	1426	OG	SER	249	-10.307	46.215	-6.203	1.00	33.59	CDK2
ATOM	1427	C	SER	249	-11.067	49.901	-6.444	1.00	33.09	CDK2
ATOM	1428	O	SER	249	-12.134	50.440	-6.130	1.00	29.78	CDK2
ATOM	1429	N	MET	250	-9.907	50.541	-6.394	1.00	27.73	CDK2
ATOM	1430	CA	MET	250	-9.884	51.920	-5.948	1.00	31.21	CDK2
ATOM	1431	CB	MET	250	-8.455	52.457	-5.918	1.00	33.74	CDK2
ATOM	1432	CG	MET	250	-8.370	53.943	-5.645	1.00	41.23	CDK2
ATOM	1433	SD	MET	250	-6.648	54.465	-5.569	1.00	48.82	CDK2
ATOM	1434	CE	MET	250	-6.298	54.631	-7.348	1.00	46.30	CDK2
ATOM	1435	C	MET	250	-10.730	52.767	-6.870	1.00	33.18	CDK2
ATOM	1436	O	MET	250	-11.505	53.597	-6.408	1.00	43.42	CDK2
ATOM	1437	N	GLY	251	-10.595	52.548	-8.178	1.00	36.22	CDK2
ATOM	1438	CA	GLY	251	-11.357	53.330	-9.142	1.00	31.16	CDK2
ATOM	1439	C	GLY	251	-12.852	53.141	-9.048	1.00	32.65	CDK2
ATOM	1440	O	GLY	251	-13.620	54.108	-9.126	1.00	34.23	CDK2
ATOM	1441	N	LEU	252	-13.271	51.886	-8.906	1.00	34.97	CDK2
ATOM	1442	CA	LEU	252	-14.690	51.570	-8.781	1.00	35.32	CDK2
ATOM	1443	CB	LEU	252	-14.868	50.046	-8.756	1.00	33.29	CDK2
ATOM	1444	CG	LEU	252	-16.116	49.372	-9.341	1.00	41.00	CDK2
ATOM	1445	CD1	LEU	252	-16.812	48.610	-8.244	1.00	30.48	CDK2
ATOM	1446	CD2	LEU	252	-17.070	50.384	-9.963	1.00	35.01	CDK2
ATOM	1447	C	LEU	252	-15.224	52.223	-7.482	1.00	38.96	CDK2
ATOM	1448	O	LEU	252	-16.303	52.831	-7.474	1.00	37.59	CDK2
ATOM	1449	N	SER	253	-14.441	52.135	-6.403	1.00	36.68	CDK2
ATOM	1450	CA	SER	253	-14.828	52.712	-5.103	1.00	41.36	CDK2
ATOM	1451	CB	SER	253	-13.783	52.382	-4.026	1.00	33.13	CDK2
ATOM	1452	OG	SER	253	-13.699	50.978	-3.838	1.00	31.56	CDK2

ATOM	1453	C	SER	253	-15.021	54.220	-5.167	1.00	40.63	CDK2
ATOM	1454	O	SER	253	-15.976	54.742	-4.605	1.00	42.49	CDK2
ATOM	1455	N	LEU	254	-14.114	54.916	-5.851	1.00	42.40	CDK2
ATOM	1456	CA	LEU	254	-14.203	56.373	-5.999	1.00	41.53	CDK2
ATOM	1457	CB	LEU	254	-12.948	56.921	-6.660	1.00	42.27	CDK2
ATOM	1458	CG	LEU	254	-11.715	57.129	-5.800	1.00	37.89	CDK2
ATOM	1459	CD1	LEU	254	-10.516	57.368	-6.708	1.00	35.93	CDK2
ATOM	1460	CD2	LEU	254	-11.944	58.304	-4.863	1.00	41.44	CDK2
ATOM	1461	C	LEU	254	-15.408	56.809	-6.828	1.00	42.25	CDK2
ATOM	1462	O	LEU	254	-15.968	57.871	-6.597	1.00	45.58	CDK2
ATOM	1463	N	VAL	255	-15.793	56.004	-7.814	1.00	48.22	CDK2
ATOM	1464	CA	VAL	255	-16.948	56.341	-8.643	1.00	48.45	CDK2
ATOM	1465	CB	VAL	255	-17.041	55.441	-9.905	1.00	50.14	CDK2
ATOM	1466	CG1	VAL	255	-18.421	55.576	-10.533	1.00	48.28	CDK2
ATOM	1467	CG2	VAL	255	-15.947	55.809	-10.911	1.00	46.02	CDK2
ATOM	1468	C	VAL	255	-18.207	56.145	-7.803	1.00	49.95	CDK2
ATOM	1469	O	VAL	255	-19.166	56.910	-7.918	1.00	51.43	CDK2
ATOM	1470	N	GLU	256	-18.205	55.110	-6.961	1.00	50.58	CDK2
ATOM	1471	CA	GLU	256	-19.354	54.841	-6.088	1.00	46.90	CDK2
ATOM	1472	CB	GLU	256	-19.160	53.548	-5.288	1.00	37.96	CDK2
ATOM	1473	CG	GLU	256	-20.244	53.354	-4.254	1.00	39.26	CDK2
ATOM	1474	CD	GLU	256	-20.210	51.996	-3.602	1.00	44.24	CDK2
ATOM	1475	OE1	GLU	256	-21.191	51.654	-2.916	1.00	45.88	CDK2
ATOM	1476	OE2	GLU	256	-19.214	51.268	-3.773	1.00	43.79	CDK2
ATOM	1477	C	GLU	256	-19.571	55.994	-5.103	1.00	48.13	CDK2
ATOM	1478	O	GLU	256	-20.681	56.526	-4.988	1.00	44.18	CDK2
ATOM	1479	N	MET	257	-18.502	56.373	-4.398	1.00	47.57	CDK2
ATOM	1480	CA	MET	257	-18.569	57.449	-3.416	1.00	48.56	CDK2
ATOM	1481	CB	MET	257	-17.233	57.558	-2.678	1.00	50.19	CDK2
ATOM	1482	CG	MET	257	-16.869	56.298	-1.901	1.00	50.08	CDK2
ATOM	1483	SD	MET	257	-15.432	56.495	-0.839	1.00	51.23	CDK2
ATOM	1484	CE	MET	257	-14.083	56.038	-1.943	1.00	48.94	CDK2
ATOM	1485	C	MET	257	-18.939	58.796	-4.031	1.00	51.94	CDK2
ATOM	1486	O	MET	257	-19.564	59.633	-3.385	1.00	52.56	CDK2
ATOM	1487	N	ALA	258	-18.553	58.998	-5.287	1.00	56.87	CDK2
ATOM	1488	CA	ALA	258	-18.847	60.240	-5.993	1.00	55.56	CDK2
ATOM	1489	CB	ALA	258	-17.894	60.398	-7.182	1.00	55.20	CDK2
ATOM	1490	C	ALA	258	-20.308	60.312	-6.463	1.00	56.01	CDK2
ATOM	1491	O	ALA	258	-20.886	61.397	-6.507	1.00	58.36	CDK2
ATOM	1492	N	VAL	259	-20.907	59.170	-6.810	1.00	53.70	CDK2
ATOM	1493	CA	VAL	259	-22.296	59.159	-7.267	1.00	54.75	CDK2
ATOM	1494	CB	VAL	259	-22.471	58.259	-8.502	1.00	52.35	CDK2
ATOM	1495	CG1	VAL	259	-21.462	58.652	-9.565	1.00	49.67	CDK2

ATOM	1496	CG2	VAL	259	-22.306	56.808	-8.118	1.00	55.21	CDK2
ATOM	1497	C	VAL	259	-23.289	58.726	-6.187	1.00	57.73	CDK2
ATOM	1498	O	VAL	259	-24.503	58.851	-6.355	1.00	59.52	CDK2
ATOM	1499	N	GLY	260	-22.770	58.225	-5.075	1.00	58.64	CDK2
ATOM	1500	CA	GLY	260	-23.634	57.803	-3.991	1.00	55.55	CDK2
ATOM	1501	C	GLY	260	-24.363	56.504	-4.238	1.00	53.40	CDK2
ATOM	1502	O	GLY	260	-25.480	56.328	-3.777	1.00	55.92	CDK2
ATOM	1503	N	ARG	261	-23.736	55.583	-4.955	1.00	56.53	CDK2
ATOM	1504	CA	ARG	261	-24.371	54.303	-5.235	1.00	57.03	CDK2
ATOM	1505	CB	ARG	261	-25.672	54.564	-5.993	1.00	64.44	CDK2
ATOM	1506	CG	ARG	261	-26.264	53.382	-6.715	1.00	67.68	CDK2
ATOM	1507	CD	ARG	261	-26.969	53.839	-7.987	1.00	69.38	CDK2
ATOM	1508	NE	ARG	261	-26.238	53.401	-9.173	1.00	78.16	CDK2
ATOM	1509	CZ	ARG	261	-26.748	53.341	-10.399	1.00	77.41	CDK2
ATOM	1510	NH1	ARG	261	-28.008	53.692	-10.626	1.00	78.33	CDK2
ATOM	1511	NH2	ARG	261	-25.990	52.920	-11.402	1.00	78.41	CDK2
ATOM	1512	C	ARG	261	-23.435	53.409	-6.047	1.00	55.57	CDK2
ATOM	1513	O	ARG	261	-22.761	53.886	-6.955	1.00	55.93	CDK2
ATOM	1514	N	TYR	262	-23.369	52.126	-5.697	1.00	52.95	CDK2
ATOM	1515	CA	TYR	262	-22.521	51.185	-6.424	1.00	49.78	CDK2
ATOM	1516	CB	TYR	262	-22.873	49.760	-6.024	1.00	43.66	CDK2
ATOM	1517	CG	TYR	262	-22.029	48.710	-6.691	1.00	39.85	CDK2
ATOM	1518	CD1	TYR	262	-20.691	48.549	-6.363	1.00	35.96	CDK2
ATOM	1519	CE1	TYR	262	-19.915	47.561	-6.972	1.00	36.69	CDK2
ATOM	1520	CD2	TYR	262	-22.579	47.862	-7.647	1.00	38.71	CDK2
ATOM	1521	CE2	TYR	262	-21.823	46.880	-8.260	1.00	36.12	CDK2
ATOM	1522	CZ	TYR	262	-20.492	46.731	-7.921	1.00	38.37	CDK2
ATOM	1523	OH	TYR	262	-19.758	45.742	-8.538	1.00	32.97	CDK2
ATOM	1524	C	TYR	262	-22.841	51.447	-7.895	1.00	51.68	CDK2
ATOM	1525	O	TYR	262	-23.978	51.293	-8.329	1.00	49.78	CDK2
ATOM	1526	N	PRO	263	-21.830	51.828	-8.680	1.00	52.54	CDK2
ATOM	1527	CD	PRO	263	-20.441	51.891	-8.200	1.00	52.60	CDK2
ATOM	1528	CA	PRO	263	-21.905	52.163	-10.106	1.00	55.43	CDK2
ATOM	1529	CB	PRO	263	-20.613	52.934	-10.331	1.00	52.93	CDK2
ATOM	1530	CG	PRO	263	-19.662	52.236	-9.455	1.00	53.90	CDK2
ATOM	1531	C	PRO	263	-22.126	51.106	-11.199	1.00	57.60	CDK2
ATOM	1532	O	PRO	263	-21.950	51.405	-12.381	1.00	57.91	CDK2
ATOM	1533	N	ILE	264	-22.494	49.883	-10.833	1.00	56.60	CDK2
ATOM	1534	CA	ILE	264	-22.737	48.860	-11.844	1.00	55.91	CDK2
ATOM	1535	CB	ILE	264	-21.646	47.767	-11.827	1.00	54.80	CDK2
ATOM	1536	CG2	ILE	264	-22.022	46.645	-12.763	1.00	53.59	CDK2
ATOM	1537	CG1	ILE	264	-20.319	48.352	-12.303	1.00	54.57	CDK2
ATOM	1538	CD1	ILE	264	-19.175	47.379	-12.250	1.00	55.31	CDK2

ATOM	1539	C	ILE	264	-24.095	48.238	-11.572	1.00	56.64	CDK2
ATOM	1540	O	ILE	264	-24.334	47.708	-10.491	1.00	57.40	CDK2
ATOM	1541	N	PRO	265	-25.008	48.289	-12.552	1.00	58.57	CDK2
ATOM	1542	CD	PRO	265	-26.375	47.784	-12.339	1.00	57.51	CDK2
ATOM	1543	CA	PRO	265	-24.867	48.874	-13.889	1.00	59.89	CDK2
ATOM	1544	CB	PRO	265	-26.095	48.364	-14.621	1.00	58.68	CDK2
ATOM	1545	CG	PRO	265	-27.118	48.294	-13.545	1.00	59.97	CDK2
ATOM	1546	C	PRO	265	-24.846	50.388	-13.855	1.00	58.62	CDK2
ATOM	1547	O	PRO	265	-25.394	50.998	-12.945	1.00	58.78	CDK2
ATOM	1548	N	PRO	266	-24.225	51.013	-14.865	1.00	59.73	CDK2
ATOM	1549	CD	PRO	266	-23.576	50.382	-16.018	1.00	60.58	CDK2
ATOM	1550	CA	PRO	266	-24.139	52.471	-14.944	1.00	60.72	CDK2
ATOM	1551	CB	PRO	266	-23.712	52.733	-16.387	1.00	59.69	CDK2
ATOM	1552	CG	PRO	266	-23.790	51.394	-17.084	1.00	61.26	CDK2
ATOM	1553	C	PRO	266	-25.463	53.137	-14.608	1.00	62.40	CDK2
ATOM	1554	O	PRO	266	-26.533	52.601	-14.891	1.00	55.48	CDK2
ATOM	1555	N	PRO	267	-25.404	54.315	-13.977	1.00	67.28	CDK2
ATOM	1556	CD	PRO	267	-24.205	55.059	-13.555	1.00	70.50	CDK2
ATOM	1557	CA	PRO	267	-26.641	55.012	-13.624	1.00	71.69	CDK2
ATOM	1558	CB	PRO	267	-26.156	56.313	-12.986	1.00	73.35	CDK2
ATOM	1559	CG	PRO	267	-24.745	56.021	-12.544	1.00	75.01	CDK2
ATOM	1560	C	PRO	267	-27.466	55.256	-14.875	1.00	74.96	CDK2
ATOM	1561	O	PRO	267	-26.850	55.614	-15.906	1.00	74.46	CDK2
ATOM	1562	OT	PRO	267	-28.701	55.076	-14.808	1.00	75.82	CDK2
ATOM	1563	CB	PRO	302	-32.709	43.995	-10.284	1.00	86.46	CDK3
ATOM	1564	CG	PRO	302	-33.660	45.170	-9.977	1.00	87.23	CDK3
ATOM	1565	C	PRO	302	-30.432	43.438	-9.344	1.00	84.52	CDK3
ATOM	1566	O	PRO	302	-29.486	43.745	-8.615	1.00	85.35	CDK3
ATOM	1567	N	PRO	302	-31.958	45.201	-8.309	1.00	88.31	CDK3
ATOM	1568	CD	PRO	302	-33.131	45.973	-8.765	1.00	88.49	CDK3
ATOM	1569	CA	PRO	302	-31.865	43.896	-9.016	1.00	87.73	CDK3
ATOM	1570	N	MET	303	-30.297	42.692	-10.439	1.00	80.45	CDK3
ATOM	1571	CA	MET	303	-29.023	42.146	-10.915	1.00	71.88	CDK3
ATOM	1572	CB	MET	303	-27.917	43.194	-10.851	1.00	72.73	CDK3
ATOM	1573	CG	MET	303	-26.717	42.836	-11.709	1.00	78.99	CDK3
ATOM	1574	SD	MET	303	-26.129	44.227	-12.694	1.00	85.97	CDK3
ATOM	1575	CE	MET	303	-26.722	43.823	-14.323	1.00	76.44	CDK3
ATOM	1576	C	MET	303	-28.578	40.879	-10.176	1.00	66.23	CDK3
ATOM	1577	O	MET	303	-28.117	40.928	-9.031	1.00	68.99	CDK3
ATOM	1578	N	ALA	304	-28.728	39.742	-10.849	1.00	55.51	CDK3
ATOM	1579	CA	ALA	304	-28.351	38.459	-10.291	1.00	42.92	CDK3
ATOM	1580	CB	ALA	304	-28.813	37.344	-11.203	1.00	42.46	CDK3
ATOM	1581	C	ALA	304	-26.847	38.401	-10.134	1.00	42.14	CDK3

ATOM	1582	O	ALA	304	-26.129	39.277	-10.604	1.00	44.69	CDK3
ATOM	1583	N	ILE	305	-26.361	37.353	-9.490	1.00	44.54	CDK3
ATOM	1584	CA	ILE	305	-24.933	37.220	-9.281	1.00	44.03	CDK3
ATOM	1585	CB	ILE	305	-24.637	35.989	-8.424	1.00	41.60	CDK3
ATOM	1586	CG2	ILE	305	-23.150	35.776	-8.325	1.00	39.49	CDK3
ATOM	1587	CG1	ILE	305	-25.247	36.193	-7.026	1.00	48.67	CDK3
ATOM	1588	CD1	ILE	305	-25.335	34.943	-6.163	1.00	45.66	CDK3
ATOM	1589	C	ILE	305	-24.188	37.147	-10.611	1.00	47.91	CDK3
ATOM	1590	O	ILE	305	-23.256	37.917	-10.853	1.00	46.71	CDK3
ATOM	1591	N	PHE	306	-24.592	36.224	-11.478	1.00	50.53	CDK3
ATOM	1592	CA	PHE	306	-23.941	36.121	-12.776	1.00	48.49	CDK3
ATOM	1593	CB	PHE	306	-24.462	34.915	-13.560	1.00	53.18	CDK3
ATOM	1594	CG	PHE	306	-23.835	34.778	-14.915	1.00	54.00	CDK3
ATOM	1595	CD1	PHE	306	-22.678	34.038	-15.080	1.00	53.50	CDK3
ATOM	1596	CD2	PHE	306	-24.361	35.455	-16.008	1.00	52.35	CDK3
ATOM	1597	CE1	PHE	306	-22.051	33.978	-16.307	1.00	56.00	CDK3
ATOM	1598	CE2	PHE	306	-23.738	35.400	-17.237	1.00	55.40	CDK3
ATOM	1599	CZ	PHE	306	-22.578	34.660	-17.388	1.00	54.98	CDK3
ATOM	1600	C	PHE	306	-24.215	37.412	-13.559	1.00	46.48	CDK3
ATOM	1601	O	PHE	306	-23.316	37.988	-14.171	1.00	42.25	CDK3
ATOM	1602	N	GLU	307	-25.461	37.870	-13.531	1.00	40.46	CDK3
ATOM	1603	CA	GLU	307	-25.821	39.095	-14.225	1.00	46.36	CDK3
ATOM	1604	CB	GLU	307	-27.251	39.488	-13.863	1.00	45.53	CDK3
ATOM	1605	CG	GLU	307	-27.717	40.748	-14.556	1.00	55.41	CDK3
ATOM	1606	CD	GLU	307	-29.202	41.028	-14.354	1.00	66.96	CDK3
ATOM	1607	OE1	GLU	307	-29.837	41.563	-15.292	1.00	70.72	CDK3
ATOM	1608	OE2	GLU	307	-29.738	40.715	-13.265	1.00	68.73	CDK3
ATOM	1609	C	GLU	307	-24.866	40.254	-13.904	1.00	49.73	CDK3
ATOM	1610	O	GLU	307	-24.495	41.023	-14.783	1.00	50.94	CDK3
ATOM	1611	N	LEU	308	-24.463	40.377	-12.643	1.00	52.65	CDK3
ATOM	1612	CA	LEU	308	-23.567	41.454	-12.223	1.00	47.13	CDK3
ATOM	1613	CB	LEU	308	-23.624	41.595	-10.689	1.00	47.72	CDK3
ATOM	1614	CG	LEU	308	-23.146	42.863	-9.963	1.00	42.73	CDK3
ATOM	1615	CD1	LEU	308	-21.684	42.732	-9.634	1.00	45.17	CDK3
ATOM	1616	CD2	LEU	308	-23.359	44.083	-10.826	1.00	49.65	CDK3
ATOM	1617	C	LEU	308	-22.114	41.234	-12.667	1.00	47.51	CDK3
ATOM	1618	O	LEU	308	-21.437	42.165	-13.131	1.00	43.11	CDK3
ATOM	1619	N	LEU	309	-21.639	40.000	-12.523	1.00	44.73	CDK3
ATOM	1620	CA	LEU	309	-20.260	39.666	-12.855	1.00	47.11	CDK3
ATOM	1621	CB	LEU	309	-19.915	38.304	-12.262	1.00	43.48	CDK3
ATOM	1622	CG	LEU	309	-19.206	38.362	-10.900	1.00	51.03	CDK3
ATOM	1623	CD1	LEU	309	-19.838	39.423	-10.017	1.00	43.46	CDK3
ATOM	1624	CD2	LEU	309	-19.264	37.003	-10.231	1.00	41.31	CDK3

ATOM	1625	C	LEU	309	-19.939	39.698	-14.348	1.00 52.38	CDK3
ATOM	1626	O	LEU	309	-18.816	40.035	-14.747	1.00 47.00	CDK3
ATOM	1627	N	ASP	310	-20.932	39.348	-15.164	1.00 56.64	CDK3
ATOM	1628	CA	ASP	310	-20.781	39.348	-16.612	1.00 56.70	CDK3
ATOM	1629	CB	ASP	310	-21.962	38.638	-17.275	1.00 62.07	CDK3
ATOM	1630	CG	ASP	310	-21.838	38.588	-18.789	1.00 69.70	CDK3
ATOM	1631	OD1	ASP	310	-20.762	38.199	-19.306	1.00 69.68	CDK3
ATOM	1632	OD2	ASP	310	-22.828	38.942	-19.463	1.00 75.42	CDK3
ATOM	1633	C	ASP	310	-20.707	40.791	-17.080	1.00 53.16	CDK3
ATOM	1634	O	ASP	310	-20.026	41.102	-18.053	1.00 54.22	CDK3
ATOM	1635	N	TYR	311	-21.392	41.671	-16.362	1.00 47.70	CDK3
ATOM	1636	CA	TYR	311	-21.384	43.079	-16.702	1.00 49.16	CDK3
ATOM	1637	CB	TYR	311	-22.475	43.823	-15.939	1.00 51.19	CDK3
ATOM	1638	CG	TYR	311	-22.757	45.177	-16.535	1.00 60.25	CDK3
ATOM	1639	CD1	TYR	311	-21.824	46.219	-16.438	1.00 61.63	CDK3
ATOM	1640	CE1	TYR	311	-22.051	47.454	-17.054	1.00 62.65	CDK3
ATOM	1641	CD2	TYR	311	-23.929	45.405	-17.256	1.00 63.40	CDK3
ATOM	1642	CE2	TYR	311	-24.167	46.631	-17.874	1.00 68.27	CDK3
ATOM	1643	CZ	TYR	311	-23.226	47.649	-17.772	1.00 67.65	CDK3
ATOM	1644	OH	TYR	311	-23.463	48.844	-18.413	1.00 71.55	CDK3
ATOM	1645	C	TYR	311	-20.044	43.765	-16.430	1.00 51.51	CDK3
ATOM	1646	O	TYR	311	-19.626	44.648	-17.179	1.00 53.84	CDK3
ATOM	1647	N	ILE	312	-19.356	43.389	-15.362	1.00 48.90	CDK3
ATOM	1648	CA	ILE	312	-18.102	44.066	-15.106	1.00 42.50	CDK3
ATOM	1649	CB	ILE	312	-17.658	43.957	-13.594	1.00 41.93	CDK3
ATOM	1650	CG2	ILE	312	-18.841	43.606	-12.691	1.00 47.16	CDK3
ATOM	1651	CG1	ILE	312	-16.572	42.906	-13.433	1.00 32.83	CDK3
ATOM	1652	CD1	ILE	312	-15.228	43.498	-13.314	1.00 32.73	CDK3
ATOM	1653	C	ILE	312	-17.017	43.545	-16.044	1.00 44.71	CDK3
ATOM	1654	O	ILE	312	-16.155	44.308	-16.475	1.00 45.76	CDK3
ATOM	1655	N	VAL	313	-17.056	42.262	-16.387	1.00 45.98	CDK3
ATOM	1656	CA	VAL	313	-16.021	41.738	-17.266	1.00 49.67	CDK3
ATOM	1657	CB	VAL	313	-15.717	40.223	-17.019	1.00 48.66	CDK3
ATOM	1658	CG1	VAL	313	-16.023	39.840	-15.589	1.00 50.93	CDK3
ATOM	1659	CG2	VAL	313	-16.497	39.363	-17.984	1.00 50.03	CDK3
ATOM	1660	C	VAL	313	-16.316	41.923	-18.752	1.00 54.76	CDK3
ATOM	1661	O	VAL	313	-15.397	42.169	-19.527	1.00 53.47	CDK3
ATOM	1662	N	ASN	314	-17.585	41.814	-19.143	1.00 56.24	CDK3
ATOM	1663	CA	ASN	314	-17.974	41.935	-20.553	1.00 56.61	CDK3
ATOM	1664	CB	ASN	314	-18.753	40.697	-20.988	1.00 48.44	CDK3
ATOM	1665	CG	ASN	314	-17.880	39.487	-21.087	1.00 53.73	CDK3
ATOM	1666	OD1	ASN	314	-18.307	38.366	-20.801	1.00 54.62	CDK3
ATOM	1667	ND2	ASN	314	-16.635	39.699	-21.487	1.00 54.50	CDK3

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ATOM   1668  C   ASN   314     -18.778  43.174 -20.944  1.00 60.24      CDK3
ATOM   1669  O   ASN   314     -19.580  43.129 -21.877  1.00 64.10      CDK3
ATOM   1670  N   GLU   315     -18.578  44.274 -20.233  1.00 59.85      CDK3
ATOM   1671  CA  GLU   315     -19.269  45.511 -20.559  1.00 56.33      CDK3
ATOM   1672  CB  GLU   315     -20.499  45.706 -19.684  1.00 48.93      CDK3
ATOM   1673  CG  GLU   315     -21.639  44.771 -20.002  1.00 58.46      CDK3
ATOM   1674  CD  GLU   315     -22.301  45.077 -21.329  1.00 64.58      CDK3
ATOM   1675  OE1 GLU   315     -22.040  46.162 -21.893  1.00 63.47      CDK3
ATOM   1676  OE2 GLU   315     -23.083  44.225 -21.804  1.00 65.68      CDK3
ATOM   1677  C   GLU   315     -18.264  46.611 -20.309  1.00 59.01      CDK3
ATOM   1678  O   GLU   315     -17.141  46.344 -19.900  1.00 57.44      CDK3
ATOM   1679  N   PRO   316     -18.650  47.865 -20.542  1.00 64.01      CDK3
ATOM   1680  CD  PRO   316     -19.949  48.384 -21.010  1.00 68.32      CDK3
ATOM   1681  CA  PRO   316     -17.683  48.939 -20.311  1.00 64.87      CDK3
ATOM   1682  CB  PRO   316     -18.210  50.075 -21.176  1.00 65.51      CDK3
ATOM   1683  CG  PRO   316     -19.702  49.875 -21.156  1.00 67.38      CDK3
ATOM   1684  C   PRO   316     -17.592  49.337 -18.853  1.00 63.28      CDK3
ATOM   1685  O   PRO   316     -18.586  49.320 -18.133  1.00 67.04      CDK3
ATOM   1686  N   PRO   317     -16.394  49.704 -18.398  1.00 59.37      CDK3
ATOM   1687  CD  PRO   317     -15.126  49.780 -19.136  1.00 58.91      CDK3
ATOM   1688  CA  PRO   317     -16.233  50.105 -17.003  1.00 60.19      CDK3
ATOM   1689  CB  PRO   317     -14.734  50.355 -16.879  1.00 59.74      CDK3
ATOM   1690  CG  PRO   317     -14.306  50.682 -18.264  1.00 59.92      CDK3
ATOM   1691  C   PRO   317     -17.038  51.371 -16.755  1.00 59.17      CDK3
ATOM   1692  O   PRO   317     -17.337  52.098 -17.690  1.00 57.29      CDK3
ATOM   1693  N   PRO   318     -17.431  51.629 -15.498  1.00 57.79      CDK3
ATOM   1694  CD  PRO   318     -17.214  50.798 -14.308  1.00 57.66      CDK3
ATOM   1695  CA  PRO   318     -18.201  52.839 -15.182  1.00 58.05      CDK3
ATOM   1696  CB  PRO   318     -18.456  52.725 -13.681  1.00 56.41      CDK3
ATOM   1697  CG  PRO   318     -18.296  51.273 -13.388  1.00 58.37      CDK3
ATOM   1698  C   PRO   318     -17.346  54.054 -15.549  1.00 60.19      CDK3
ATOM   1699  O   PRO   318     -16.158  53.898 -15.848  1.00 60.33      CDK3
ATOM   1700  N   LYS   319     -17.912  55.258 -15.506  1.00 61.87      CDK3
ATOM   1701  CA  LYS   319     -17.133  56.415 -15.929  1.00 67.58      CDK3
ATOM   1702  CB  LYS   319     -17.496  56.763 -17.383  1.00 69.91      CDK3
ATOM   1703  CG  LYS   319     -16.684  56.014 -18.444  1.00 77.10      CDK3
ATOM   1704  CD  LYS   319     -16.479  56.855 -19.709  1.00 81.25      CDK3
ATOM   1705  CE  LYS   319     -17.570  56.601 -20.752  1.00 83.69      CDK3
ATOM   1706  NZ  LYS   319     -18.952  56.833 -20.231  1.00 77.88      CDK3
ATOM   1707  C   LYS   319     -17.162  57.696 -15.116  1.00 68.31      CDK3
ATOM   1708  O   LYS   319     -16.170  58.434 -15.115  1.00 73.00      CDK3
ATOM   1709  N   LEU   320     -18.280  57.974 -14.449  1.00 66.44      CDK3
ATOM   1710  CA  LEU   320     -18.440  59.208 -13.665  1.00 69.03      CDK3
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ATOM	1711	CB	LEU	320	-17.076	59.747	-13.197	1.00	62.36	CDK3
ATOM	1712	CG	LEU	320	-16.941	60.534	-11.894	1.00	61.94	CDK3
ATOM	1713	CD1	LEU	320	-17.519	59.720	-10.752	1.00	60.53	CDK3
ATOM	1714	CD2	LEU	320	-15.467	60.850	-11.630	1.00	54.68	CDK3
ATOM	1715	C	LEU	320	-19.119	60.251	-14.565	1.00	72.44	CDK3
ATOM	1716	O	LEU	320	-18.556	60.651	-15.589	1.00	75.34	CDK3
ATOM	1717	N	PRO	321	-20.336	60.701	-14.204	1.00	73.29	CDK3
ATOM	1718	CD	PRO	321	-21.119	60.346	-13.012	1.00	74.03	CDK3
ATOM	1719	CA	PRO	321	-21.039	61.699	-15.021	1.00	74.68	CDK3
ATOM	1720	CB	PRO	321	-22.192	62.166	-14.124	1.00	74.13	CDK3
ATOM	1721	CG	PRO	321	-21.902	61.599	-12.765	1.00	73.85	CDK3
ATOM	1722	C	PRO	321	-20.129	62.855	-15.412	1.00	75.85	CDK3
ATOM	1723	O	PRO	321	-19.131	63.115	-14.746	1.00	77.46	CDK3
ATOM	1724	N	SER	322	-20.463	63.545	-16.496	1.00	77.94	CDK3
ATOM	1725	CA	SER	322	-19.643	64.671	-16.915	1.00	77.74	CDK3
ATOM	1726	CB	SER	322	-19.391	64.636	-18.424	1.00	78.27	CDK3
ATOM	1727	OG	SER	322	-18.450	65.636	-18.786	1.00	77.21	CDK3
ATOM	1728	C	SER	322	-20.280	66.000	-16.541	1.00	76.63	CDK3
ATOM	1729	O	SER	322	-21.478	66.079	-16.241	1.00	72.22	CDK3
ATOM	1730	N	GLY	323	-19.461	67.045	-16.556	1.00	76.88	CDK3
ATOM	1731	CA	GLY	323	-19.951	68.366	-16.221	1.00	80.16	CDK3
ATOM	1732	C	GLY	323	-20.176	68.540	-14.736	1.00	80.63	CDK3
ATOM	1733	O	GLY	323	-20.085	69.654	-14.215	1.00	82.68	CDK3
ATOM	1734	N	VAL	324	-20.480	67.439	-14.054	1.00	79.42	CDK3
ATOM	1735	CA	VAL	324	-20.705	67.468	-12.614	1.00	75.52	CDK3
ATOM	1736	CB	VAL	324	-21.668	66.332	-12.170	1.00	75.24	CDK3
ATOM	1737	CG1	VAL	324	-22.182	66.611	-10.770	1.00	72.71	CDK3
ATOM	1738	CG2	VAL	324	-22.831	66.206	-13.153	1.00	72.54	CDK3
ATOM	1739	C	VAL	324	-19.357	67.299	-11.900	1.00	74.32	CDK3
ATOM	1740	O	VAL	324	-19.203	67.691	-10.740	1.00	74.18	CDK3
ATOM	1741	N	PHE	325	-18.386	66.724	-12.612	1.00	70.26	CDK3
ATOM	1742	CA	PHE	325	-17.047	66.487	-12.074	1.00	67.49	CDK3
ATOM	1743	CB	PHE	325	-16.828	64.995	-11.800	1.00	62.60	CDK3
ATOM	1744	CG	PHE	325	-17.766	64.424	-10.793	1.00	57.28	CDK3
ATOM	1745	CD1	PHE	325	-17.520	64.575	-9.435	1.00	49.48	CDK3
ATOM	1746	CD2	PHE	325	-18.909	63.743	-11.202	1.00	54.27	CDK3
ATOM	1747	CE1	PHE	325	-18.406	64.051	-8.496	1.00	52.93	CDK3
ATOM	1748	CE2	PHE	325	-19.802	63.215	-10.269	1.00	53.02	CDK3
ATOM	1749	CZ	PHE	325	-19.552	63.368	-8.914	1.00	47.52	CDK3
ATOM	1750	C	PHE	325	-15.951	66.963	-13.019	1.00	67.59	CDK3
ATOM	1751	O	PHE	325	-16.044	66.797	-14.239	1.00	66.10	CDK3
ATOM	1752	N	SER	326	-14.901	67.529	-12.433	1.00	67.53	CDK3
ATOM	1753	CA	SER	326	-13.763	68.036	-13.182	1.00	65.24	CDK3

ATOM	1754	CB	SER	326	-12.653	68.452	-12.223	1.00	63.35	CDK3
ATOM	1755	OG	SER	326	-11.512	67.639	-12.412	1.00	65.72	CDK3
ATOM	1756	C	SER	326	-13.217	67.010	-14.167	1.00	65.84	CDK3
ATOM	1757	O	SER	326	-13.314	65.805	-13.947	1.00	66.77	CDK3
ATOM	1758	N	LEU	327	-12.643	67.507	-15.255	1.00	66.25	CDK3
ATOM	1759	CA	LEU	327	-12.072	66.659	-16.285	1.00	66.92	CDK3
ATOM	1760	CB	LEU	327	-11.536	67.517	-17.438	1.00	67.30	CDK3
ATOM	1761	CG	LEU	327	-12.411	67.859	-18.655	1.00	67.99	CDK3
ATOM	1762	CD1	LEU	327	-11.860	67.113	-19.855	1.00	66.89	CDK3
ATOM	1763	CD2	LEU	327	-13.879	67.506	-18.424	1.00	65.62	CDK3
ATOM	1764	C	LEU	327	-10.938	65.843	-15.687	1.00	67.57	CDK3
ATOM	1765	O	LEU	327	-10.750	64.682	-16.052	1.00	68.43	CDK3
ATOM	1766	N	GLU	328	-10.184	66.458	-14.775	1.00	66.69	CDK3
ATOM	1767	CA	GLU	328	-9.057	65.798	-14.112	1.00	67.49	CDK3
ATOM	1768	CB	GLU	328	-8.425	66.735	-13.089	1.00	70.05	CDK3
ATOM	1769	CG	GLU	328	-7.028	67.192	-13.450	1.00	79.69	CDK3
ATOM	1770	CD	GLU	328	-6.909	68.708	-13.487	1.00	84.86	CDK3
ATOM	1771	OE1	GLU	328	-5.766	69.224	-13.411	1.00	87.51	CDK3
ATOM	1772	OE2	GLU	328	-7.963	69.380	-13.593	1.00	84.88	CDK3
ATOM	1773	C	GLU	328	-9.496	64.521	-13.399	1.00	68.12	CDK3
ATOM	1774	O	GLU	328	-8.926	63.447	-13.611	1.00	65.67	CDK3
ATOM	1775	N	PHE	329	-10.501	64.657	-12.538	1.00	66.93	CDK3
ATOM	1776	CA	PHE	329	-11.046	63.535	-11.786	1.00	65.84	CDK3
ATOM	1777	CB	PHE	329	-12.213	64.019	-10.918	1.00	65.11	CDK3
ATOM	1778	CG	PHE	329	-12.771	62.978	-9.982	1.00	62.51	CDK3
ATOM	1779	CD1	PHE	329	-12.026	61.866	-9.615	1.00	62.91	CDK3
ATOM	1780	CD2	PHE	329	-14.050	63.130	-9.453	1.00	61.41	CDK3
ATOM	1781	CE1	PHE	329	-12.546	60.927	-8.739	1.00	62.91	CDK3
ATOM	1782	CE2	PHE	329	-14.577	62.198	-8.578	1.00	58.95	CDK3
ATOM	1783	CZ	PHE	329	-13.826	61.094	-8.219	1.00	62.24	CDK3
ATOM	1784	C	PHE	329	-11.520	62.464	-12.764	1.00	67.41	CDK3
ATOM	1785	O	PHE	329	-11.185	61.291	-12.624	1.00	72.63	CDK3
ATOM	1786	N	GLN	330	-12.286	62.867	-13.769	1.00	63.92	CDK3
ATOM	1787	CA	GLN	330	-12.785	61.912	-14.743	1.00	62.78	CDK3
ATOM	1788	CB	GLN	330	-13.567	62.651	-15.835	1.00	63.85	CDK3
ATOM	1789	CG	GLN	330	-14.785	63.409	-15.299	1.00	63.25	CDK3
ATOM	1790	CD	GLN	330	-15.671	63.976	-16.401	1.00	64.19	CDK3
ATOM	1791	OE1	GLN	330	-16.151	65.112	-16.314	1.00	64.08	CDK3
ATOM	1792	NE2	GLN	330	-15.891	63.186	-17.442	1.00	59.25	CDK3
ATOM	1793	C	GLN	330	-11.656	61.065	-15.343	1.00	61.76	CDK3
ATOM	1794	O	GLN	330	-11.765	59.836	-15.407	1.00	60.76	CDK3
ATOM	1795	N	ASP	331	-10.572	61.714	-15.764	1.00	61.24	CDK3
ATOM	1796	CA	ASP	331	-9.427	61.005	-16.348	1.00	62.03	CDK3

ATOM	1797	CB	ASP	331	-8.323	61.990	-16.774	1.00	66.28	CDK3
ATOM	1798	CG	ASP	331	-7.212	61.321	-17.592	1.00	66.50	CDK3
ATOM	1799	OD1	ASP	331	-7.508	60.793	-18.686	1.00	62.76	CDK3
ATOM	1800	OD2	ASP	331	-6.043	61.321	-17.144	1.00	65.92	CDK3
ATOM	1801	C	ASP	331	-8.849	60.022	-15.343	1.00	60.53	CDK3
ATOM	1802	O	ASP	331	-8.621	58.854	-15.664	1.00	64.37	CDK3
ATOM	1803	N	PHE	332	-8.607	60.507	-14.128	1.00	56.58	CDK3
ATOM	1804	CA	PHE	332	-8.058	59.675	-13.060	1.00	55.06	CDK3
ATOM	1805	CB	PHE	332	-8.059	60.454	-11.741	1.00	51.63	CDK3
ATOM	1806	CG	PHE	332	-7.404	59.727	-10.610	1.00	55.37	CDK3
ATOM	1807	CD1	PHE	332	-8.174	59.069	-9.649	1.00	54.90	CDK3
ATOM	1808	CD2	PHE	332	-6.021	59.683	-10.507	1.00	54.18	CDK3
ATOM	1809	CE1	PHE	332	-7.576	58.378	-8.603	1.00	55.50	CDK3
ATOM	1810	CE2	PHE	332	-5.409	58.992	-9.462	1.00	55.56	CDK3
ATOM	1811	CZ	PHE	332	-6.190	58.338	-8.508	1.00	57.42	CDK3
ATOM	1812	C	PHE	332	-8.856	58.373	-12.910	1.00	51.32	CDK3
ATOM	1813	O	PHE	332	-8.301	57.282	-13.019	1.00	48.95	CDK3
ATOM	1814	N	VAL	333	-10.158	58.504	-12.674	1.00	49.39	CDK3
ATOM	1815	CA	VAL	333	-11.043	57.361	-12.512	1.00	47.74	CDK3
ATOM	1816	CB	VAL	333	-12.501	57.811	-12.392	1.00	47.02	CDK3
ATOM	1817	CG1	VAL	333	-13.427	56.704	-12.850	1.00	54.16	CDK3
ATOM	1818	CG2	VAL	333	-12.803	58.203	-10.968	1.00	48.30	CDK3
ATOM	1819	C	VAL	333	-10.927	56.479	-13.737	1.00	50.98	CDK3
ATOM	1820	O	VAL	333	-10.777	55.257	-13.637	1.00	53.45	CDK3
ATOM	1821	N	ASN	334	-10.992	57.113	-14.901	1.00	52.37	CDK3
ATOM	1822	CA	ASN	334	-10.917	56.390	-16.153	1.00	51.49	CDK3
ATOM	1823	CB	ASN	334	-11.146	57.356	-17.312	1.00	58.32	CDK3
ATOM	1824	CG	ASN	334	-12.620	57.524	-17.638	1.00	64.24	CDK3
ATOM	1825	OD1	ASN	334	-13.356	58.215	-16.922	1.00	69.23	CDK3
ATOM	1826	ND2	ASN	334	-13.064	56.880	-18.715	1.00	67.90	CDK3
ATOM	1827	C	ASN	334	-9.618	55.605	-16.339	1.00	49.64	CDK3
ATOM	1828	O	ASN	334	-9.625	54.525	-16.943	1.00	50.44	CDK3
ATOM	1829	N	LYS	335	-8.516	56.130	-15.808	1.00	46.50	CDK3
ATOM	1830	CA	LYS	335	-7.221	55.465	-15.917	1.00	46.70	CDK3
ATOM	1831	CB	LYS	335	-6.102	56.456	-15.596	1.00	51.90	CDK3
ATOM	1832	CG	LYS	335	-6.121	57.710	-16.450	1.00	49.82	CDK3
ATOM	1833	CD	LYS	335	-4.707	58.229	-16.698	1.00	60.79	CDK3
ATOM	1834	CE	LYS	335	-4.267	58.023	-18.149	1.00	64.53	CDK3
ATOM	1835	NZ	LYS	335	-5.140	58.762	-19.107	1.00	62.26	CDK3
ATOM	1836	C	LYS	335	-7.116	54.250	-14.989	1.00	46.99	CDK3
ATOM	1837	O	LYS	335	-6.271	53.367	-15.191	1.00	44.82	CDK3
ATOM	1838	N	CYS	336	-7.978	54.226	-13.974	1.00	44.91	CDK3
ATOM	1839	CA	CYS	336	-8.023	53.143	-12.995	1.00	48.98	CDK3

ATOM	1840	CB	CYS	336	-8.580	53.635	-11.651	1.00	45.66	CDK3
ATOM	1841	SG	CYS	336	-7.634	54.878	-10.799	1.00	44.56	CDK3
ATOM	1842	C	CYS	336	-8.959	52.058	-13.487	1.00	50.12	CDK3
ATOM	1843	O	CYS	336	-8.739	50.876	-13.231	1.00	48.67	CDK3
ATOM	1844	N	LEU	337	-10.018	52.475	-14.180	1.00	50.05	CDK3
ATOM	1845	CA	LEU	337	-11.026	51.540	-14.659	1.00	45.46	CDK3
ATOM	1846	CB	LEU	337	-12.407	52.194	-14.541	1.00	40.38	CDK3
ATOM	1847	CG	LEU	337	-12.749	52.535	-13.070	1.00	41.93	CDK3
ATOM	1848	CD1	LEU	337	-14.092	53.253	-12.953	1.00	39.02	CDK3
ATOM	1849	CD2	LEU	337	-12.781	51.239	-12.257	1.00	30.55	CDK3
ATOM	1850	C	LEU	337	-10.794	50.961	-16.049	1.00	50.11	CDK3
ATOM	1851	O	LEU	337	-11.740	50.554	-16.730	1.00	50.94	CDK3
ATOM	1852	N	ILE	338	-9.525	50.911	-16.455	1.00	49.86	CDK3
ATOM	1853	CA	ILE	338	-9.135	50.346	-17.743	1.00	47.57	CDK3
ATOM	1854	CB	ILE	338	-7.707	50.783	-18.157	1.00	49.83	CDK3
ATOM	1855	CG2	ILE	338	-7.169	49.850	-19.223	1.00	48.39	CDK3
ATOM	1856	CG1	ILE	338	-7.722	52.214	-18.698	1.00	52.52	CDK3
ATOM	1857	CD1	ILE	338	-6.339	52.810	-18.861	1.00	55.57	CDK3
ATOM	1858	C	ILE	338	-9.132	48.830	-17.559	1.00	49.51	CDK3
ATOM	1859	O	ILE	338	-8.327	48.290	-16.804	1.00	49.16	CDK3
ATOM	1860	N	LYS	339	-10.026	48.143	-18.252	1.00	47.94	CDK3
ATOM	1861	CA	LYS	339	-10.114	46.701	-18.129	1.00	47.62	CDK3
ATOM	1862	CB	LYS	339	-11.038	46.154	-19.198	1.00	44.94	CDK3
ATOM	1863	CG	LYS	339	-12.464	46.017	-18.745	1.00	49.15	CDK3
ATOM	1864	CD	LYS	339	-12.942	44.597	-18.996	1.00	45.51	CDK3
ATOM	1865	CE	LYS	339	-14.254	44.623	-19.740	1.00	50.34	CDK3
ATOM	1866	NZ	LYS	339	-15.033	45.805	-19.331	1.00	50.54	CDK3
ATOM	1867	C	LYS	339	-8.795	45.939	-18.166	1.00	47.28	CDK3
ATOM	1868	O	LYS	339	-8.626	44.973	-17.428	1.00	52.56	CDK3
ATOM	1869	N	ASN	340	-7.856	46.346	-19.009	1.00	46.97	CDK3
ATOM	1870	CA	ASN	340	-6.589	45.622	-19.084	1.00	43.38	CDK3
ATOM	1871	CB	ASN	340	-5.962	45.774	-20.463	1.00	40.09	CDK3
ATOM	1872	CG	ASN	340	-4.780	44.865	-20.647	1.00	41.43	CDK3
ATOM	1873	OD1	ASN	340	-4.896	43.806	-21.245	1.00	51.43	CDK3
ATOM	1874	ND2	ASN	340	-3.635	45.262	-20.113	1.00	44.36	CDK3
ATOM	1875	C	ASN	340	-5.595	46.073	-18.018	1.00	43.08	CDK3
ATOM	1876	O	ASN	340	-5.225	47.253	-17.951	1.00	45.44	CDK3
ATOM	1877	N	PRO	341	-5.114	45.123	-17.198	1.00	39.50	CDK3
ATOM	1878	CD	PRO	341	-5.465	43.701	-17.339	1.00	36.93	CDK3
ATOM	1879	CA	PRO	341	-4.159	45.360	-16.099	1.00	40.45	CDK3
ATOM	1880	CB	PRO	341	-3.879	43.960	-15.532	1.00	39.10	CDK3
ATOM	1881	CG	PRO	341	-4.971	43.091	-16.045	1.00	38.89	CDK3
ATOM	1882	C	PRO	341	-2.871	46.083	-16.479	1.00	41.90	CDK3

ATOM	1883	O	PRO	341	-2.497	47.076	-15.844	1.00	38.80	CDK3
ATOM	1884	N	ALA	342	-2.197	45.579	-17.513	1.00	44.17	CDK3
ATOM	1885	CA	ALA	342	-0.938	46.164	-17.987	1.00	39.97	CDK3
ATOM	1886	CB	ALA	342	-0.326	45.265	-19.031	1.00	37.41	CDK3
ATOM	1887	C	ALA	342	-1.181	47.565	-18.548	1.00	38.44	CDK3
ATOM	1888	O	ALA	342	-0.390	48.498	-18.345	1.00	37.55	CDK3
ATOM	1889	N	ALA	343	-2.303	47.727	-19.223	1.00	38.73	CDK3
ATOM	1890	CA	ALA	343	-2.633	49.026	-19.775	1.00	42.83	CDK3
ATOM	1891	CB	ALA	343	-3.782	48.895	-20.782	1.00	42.19	CDK3
ATOM	1892	C	ALA	343	-3.019	49.965	-18.637	1.00	44.61	CDK3
ATOM	1893	O	ALA	343	-2.545	51.097	-18.569	1.00	50.37	CDK3
ATOM	1894	N	ARG	344	-3.881	49.489	-17.742	1.00	43.91	CDK3
ATOM	1895	CA	ARG	344	-4.335	50.285	-16.600	1.00	41.14	CDK3
ATOM	1896	CB	ARG	344	-4.993	49.373	-15.564	1.00	44.20	CDK3
ATOM	1897	CG	ARG	344	-5.750	50.092	-14.457	1.00	40.28	CDK3
ATOM	1898	CD	ARG	344	-6.904	49.209	-13.965	1.00	37.88	CDK3
ATOM	1899	NE	ARG	344	-6.456	47.911	-13.480	1.00	29.47	CDK3
ATOM	1900	CZ	ARG	344	-7.039	46.762	-13.782	1.00	36.21	CDK3
ATOM	1901	NH1	ARG	344	-8.092	46.746	-14.572	1.00	40.12	CDK3
ATOM	1902	NH2	ARG	344	-6.592	45.626	-13.266	1.00	40.45	CDK3
ATOM	1903	C	ARG	344	-3.175	50.998	-15.943	1.00	31.00	CDK3
ATOM	1904	O	ARG	344	-2.076	50.454	-15.873	1.00	35.63	CDK3
ATOM	1905	N	ALA	345	-3.405	52.215	-15.470	1.00	29.43	CDK3
ATOM	1906	CA	ALA	345	-2.345	52.946	-14.779	1.00	32.63	CDK3
ATOM	1907	CB	ALA	345	-2.816	54.332	-14.381	1.00	29.32	CDK3
ATOM	1908	C	ALA	345	-1.938	52.179	-13.526	1.00	38.92	CDK3
ATOM	1909	O	ALA	345	-2.698	51.357	-12.994	1.00	36.34	CDK3
ATOM	1910	N	ASP	346	-0.735	52.461	-13.056	1.00	39.04	CDK3
ATOM	1911	CA	ASP	346	-0.221	51.825	-11.866	1.00	44.89	CDK3
ATOM	1912	CB	ASP	346	1.057	51.053	-12.210	1.00	41.80	CDK3
ATOM	1913	CG	ASP	346	2.262	51.959	-12.361	1.00	44.19	CDK3
ATOM	1914	OD1	ASP	346	2.077	53.181	-12.580	1.00	40.15	CDK3
ATOM	1915	OD2	ASP	346	3.397	51.445	-12.253	1.00	46.57	CDK3
ATOM	1916	C	ASP	346	0.031	52.920	-10.811	1.00	47.78	CDK3
ATOM	1917	O	ASP	346	-0.171	54.107	-11.085	1.00	52.73	CDK3
ATOM	1918	N	LEU	347	0.465	52.523	-9.618	1.00	47.31	CDK3
ATOM	1919	CA	LEU	347	0.706	53.460	-8.515	1.00	46.91	CDK3
ATOM	1920	CB	LEU	347	1.277	52.702	-7.299	1.00	40.94	CDK3
ATOM	1921	CG	LEU	347	0.344	52.212	-6.184	1.00	37.81	CDK3
ATOM	1922	CD1	LEU	347	-1.074	52.386	-6.571	1.00	33.79	CDK3
ATOM	1923	CD2	LEU	347	0.622	50.760	-5.872	1.00	37.80	CDK3
ATOM	1924	C	LEU	347	1.618	54.633	-8.872	1.00	44.46	CDK3
ATOM	1925	O	LEU	347	1.295	55.783	-8.580	1.00	46.76	CDK3

ATOM	1926	N	LYS	348	2.751	54.337	-9.498	1.00	45.69	CDK3
ATOM	1927	CA	LYS	348	3.723	55.355	-9.903	1.00	49.70	CDK3
ATOM	1928	CB	LYS	348	4.795	54.726	-10.790	1.00	55.43	CDK3
ATOM	1929	CG	LYS	348	6.133	54.498	-10.104	1.00	68.59	CDK3
ATOM	1930	CD	LYS	348	6.534	53.012	-10.102	1.00	78.68	CDK3
ATOM	1931	CE	LYS	348	7.100	52.555	-11.453	1.00	79.23	CDK3
ATOM	1932	NZ	LYS	348	6.899	51.084	-11.687	1.00	80.86	CDK3
ATOM	1933	C	LYS	348	3.094	56.507	-10.674	1.00	50.42	CDK3
ATOM	1934	O	LYS	348	3.322	57.678	-10.373	1.00	45.05	CDK3
ATOM	1935	N	GLN	349	2.308	56.158	-11.686	1.00	51.91	CDK3
ATOM	1936	CA	GLN	349	1.668	57.153	-12.527	1.00	52.37	CDK3
ATOM	1937	CB	GLN	349	1.161	56.503	-13.802	1.00	49.90	CDK3
ATOM	1938	CG	GLN	349	2.261	55.846	-14.623	1.00	52.77	CDK3
ATOM	1939	CD	GLN	349	1.698	54.977	-15.724	1.00	51.44	CDK3
ATOM	1940	OE1	GLN	349	0.505	54.698	-15.742	1.00	57.40	CDK3
ATOM	1941	NE2	GLN	349	2.551	54.544	-16.647	1.00	56.98	CDK3
ATOM	1942	C	GLN	349	0.541	57.899	-11.848	1.00	55.12	CDK3
ATOM	1943	O	GLN	349	0.505	59.129	-11.882	1.00	57.70	CDK3
ATOM	1944	N	LEU	350	-0.386	57.169	-11.237	1.00	55.29	CDK3
ATOM	1945	CA	LEU	350	-1.495	57.827	-10.556	1.00	51.73	CDK3
ATOM	1946	CB	LEU	350	-2.358	56.802	-9.802	1.00	50.66	CDK3
ATOM	1947	CG	LEU	350	-3.181	55.786	-10.605	1.00	51.30	CDK3
ATOM	1948	CD1	LEU	350	-3.905	54.853	-9.641	1.00	47.33	CDK3
ATOM	1949	CD2	LEU	350	-4.182	56.502	-11.500	1.00	43.67	CDK3
ATOM	1950	C	LEU	350	-0.920	58.856	-9.577	1.00	52.44	CDK3
ATOM	1951	O	LEU	350	-1.514	59.911	-9.365	1.00	48.13	CDK3
ATOM	1952	N	MET	351	0.241	58.554	-8.995	1.00	54.29	CDK3
ATOM	1953	CA	MET	351	0.872	59.467	-8.041	1.00	60.35	CDK3
ATOM	1954	CB	MET	351	2.154	58.861	-7.452	1.00	62.76	CDK3
ATOM	1955	CG	MET	351	1.952	57.989	-6.213	1.00	72.22	CDK3
ATOM	1956	SD	MET	351	2.080	58.836	-4.606	1.00	77.14	CDK3
ATOM	1957	CE	MET	351	1.030	60.277	-4.886	1.00	71.16	CDK3
ATOM	1958	C	MET	351	1.225	60.798	-8.686	1.00	61.25	CDK3
ATOM	1959	O	MET	351	1.205	61.838	-8.031	1.00	64.89	CDK3
ATOM	1960	N	VAL	352	1.566	60.768	-9.967	1.00	60.15	CDK3
ATOM	1961	CA	VAL	352	1.929	61.992	-10.660	1.00	59.41	CDK3
ATOM	1962	CB	VAL	352	3.189	61.790	-11.532	1.00	59.52	CDK3
ATOM	1963	CG1	VAL	352	4.307	61.198	-10.689	1.00	52.11	CDK3
ATOM	1964	CG2	VAL	352	2.873	60.885	-12.725	1.00	56.42	CDK3
ATOM	1965	C	VAL	352	0.800	62.504	-11.537	1.00	62.49	CDK3
ATOM	1966	O	VAL	352	1.002	63.430	-12.318	1.00	63.78	CDK3
ATOM	1967	N	HIS	353	-0.387	61.910	-11.404	1.00	61.50	CDK3
ATOM	1968	CA	HIS	353	-1.545	62.317	-12.200	1.00	55.52	CDK3

ATOM	1969	CB	HIS	353	-2.687	61.318	-12.040	1.00	50.17	CDK3
ATOM	1970	CG	HIS	353	-3.809	61.510	-13.017	1.00	45.39	CDK3
ATOM	1971	CD2	HIS	353	-4.142	60.824	-14.136	1.00	36.04	CDK3
ATOM	1972	ND1	HIS	353	-4.780	62.479	-12.859	1.00	42.68	CDK3
ATOM	1973	CE1	HIS	353	-5.664	62.378	-13.836	1.00	42.75	CDK3
ATOM	1974	NE2	HIS	353	-5.299	61.382	-14.624	1.00	43.30	CDK3
ATOM	1975	C	HIS	353	-2.032	63.697	-11.809	1.00	59.50	CDK3
ATOM	1976	O	HIS	353	-1.936	64.099	-10.653	1.00	59.36	CDK3
ATOM	1977	N	ALA	354	-2.564	64.417	-12.787	1.00	62.49	CDK3
ATOM	1978	CA	ALA	354	-3.055	65.765	-12.559	1.00	63.74	CDK3
ATOM	1979	CB	ALA	354	-3.707	66.301	-13.820	1.00	63.53	CDK3
ATOM	1980	C	ALA	354	-4.033	65.851	-11.406	1.00	66.04	CDK3
ATOM	1981	O	ALA	354	-3.900	66.718	-10.542	1.00	69.66	CDK3
ATOM	1982	N	PHE	355	-5.017	64.957	-11.389	1.00	66.02	CDK3
ATOM	1983	CA	PHE	355	-6.030	64.987	-10.339	1.00	64.52	CDK3
ATOM	1984	CB	PHE	355	-6.968	63.784	-10.448	1.00	64.76	CDK3
ATOM	1985	CG	PHE	355	-8.006	63.741	-9.367	1.00	64.48	CDK3
ATOM	1986	CD1	PHE	355	-9.058	64.657	-9.361	1.00	67.82	CDK3
ATOM	1987	CD2	PHE	355	-7.916	62.813	-8.330	1.00	62.22	CDK3
ATOM	1988	CE1	PHE	355	-10.009	64.653	-8.337	1.00	65.40	CDK3
ATOM	1989	CE2	PHE	355	-8.858	62.799	-7.303	1.00	61.94	CDK3
ATOM	1990	CZ	PHE	355	-9.907	63.722	-7.306	1.00	63.76	CDK3
ATOM	1991	C	PHE	355	-5.466	65.056	-8.927	1.00	59.23	CDK3
ATOM	1992	O	PHE	355	-5.910	65.865	-8.116	1.00	60.18	CDK3
ATOM	1993	N	ILE	356	-4.494	64.216	-8.615	1.00	57.62	CDK3
ATOM	1994	CA	ILE	356	-3.960	64.269	-7.275	1.00	57.94	CDK3
ATOM	1995	CB	ILE	356	-3.260	62.941	-6.865	1.00	57.42	CDK3
ATOM	1996	CG2	ILE	356	-4.084	61.754	-7.322	1.00	56.22	CDK3
ATOM	1997	CG1	ILE	356	-1.843	62.890	-7.407	1.00	55.36	CDK3
ATOM	1998	CD1	ILE	356	-0.830	62.824	-6.303	1.00	56.28	CDK3
ATOM	1999	C	ILE	356	-3.032	65.460	-7.113	1.00	59.61	CDK3
ATOM	2000	O	ILE	356	-3.049	66.106	-6.068	1.00	65.47	CDK3
ATOM	2001	N	LYS	357	-2.241	65.778	-8.139	1.00	60.51	CDK3
ATOM	2002	CA	LYS	357	-1.334	66.934	-8.064	1.00	56.57	CDK3
ATOM	2003	CB	LYS	357	-0.580	67.120	-9.382	1.00	57.29	CDK3
ATOM	2004	CG	LYS	357	0.578	66.149	-9.567	1.00	59.80	CDK3
ATOM	2005	CD	LYS	357	1.670	66.745	-10.442	1.00	66.45	CDK3
ATOM	2006	CE	LYS	357	3.066	66.350	-9.945	1.00	71.83	CDK3
ATOM	2007	NZ	LYS	357	3.904	67.531	-9.542	1.00	69.60	CDK3
ATOM	2008	C	LYS	357	-2.143	68.186	-7.743	1.00	54.93	CDK3
ATOM	2009	O	LYS	357	-1.755	68.988	-6.896	1.00	52.41	CDK3
ATOM	2010	N	ARG	358	-3.270	68.347	-8.427	1.00	55.98	CDK3
ATOM	2011	CA	ARG	358	-4.151	69.478	-8.180	1.00	59.41	CDK3

ATOM	2012	CB	ARG	358	-5.146	69.673	-9.336	1.00	60.96	CDK3
ATOM	2013	CG	ARG	358	-6.313	70.624	-9.000	1.00	64.19	CDK3
ATOM	2014	CD	ARG	358	-7.653	70.211	-9.639	1.00	66.39	CDK3
ATOM	2015	NE	ARG	358	-8.532	69.492	-8.711	1.00	68.46	CDK3
ATOM	2016	CZ	ARG	358	-9.584	68.763	-9.081	1.00	68.21	CDK3
ATOM	2017	NH1	ARG	358	-9.897	68.653	-10.365	1.00	68.26	CDK3
ATOM	2018	NH2	ARG	358	-10.317	68.130	-8.172	1.00	66.20	CDK3
ATOM	2019	C	ARG	358	-4.927	69.187	-6.903	1.00	61.53	CDK3
ATOM	2020	O	ARG	358	-5.579	70.068	-6.351	1.00	62.91	CDK3
ATOM	2021	N	SER	359	-4.849	67.944	-6.433	1.00	65.16	CDK3
ATOM	2022	CA	SER	359	-5.569	67.546	-5.228	1.00	67.90	CDK3
ATOM	2023	CB	SER	359	-6.055	66.104	-5.360	1.00	65.86	CDK3
ATOM	2024	OG	SER	359	-7.135	65.875	-4.483	1.00	66.18	CDK3
ATOM	2025	C	SER	359	-4.793	67.710	-3.922	1.00	67.73	CDK3
ATOM	2026	O	SER	359	-5.300	68.310	-2.976	1.00	67.64	CDK3
ATOM	2027	N	ASP	360	-3.577	67.178	-3.849	1.00	70.10	CDK3
ATOM	2028	CA	ASP	360	-2.801	67.323	-2.620	1.00	74.70	CDK3
ATOM	2029	CB	ASP	360	-1.675	66.280	-2.527	1.00	74.92	CDK3
ATOM	2030	CG	ASP	360	-0.813	66.234	-3.761	1.00	73.84	CDK3
ATOM	2031	OD1	ASP	360	-1.205	66.843	-4.776	1.00	75.39	CDK3
ATOM	2032	OD2	ASP	360	0.257	65.585	-3.716	1.00	69.92	CDK3
ATOM	2033	C	ASP	360	-2.220	68.723	-2.538	1.00	76.36	CDK3
ATOM	2034	O	ASP	360	-1.311	68.992	-1.755	1.00	76.36	CDK3
ATOM	2035	N	ALA	361	-2.761	69.611	-3.363	1.00	79.94	CDK3
ATOM	2036	CA	ALA	361	-2.343	71.000	-3.396	1.00	80.32	CDK3
ATOM	2037	CB	ALA	361	-1.696	71.321	-4.729	1.00	78.83	CDK3
ATOM	2038	C	ALA	361	-3.598	71.834	-3.205	1.00	82.57	CDK3
ATOM	2039	O	ALA	361	-3.719	72.922	-3.756	1.00	86.26	CDK3
ATOM	2040	N	GLU	362	-4.537	71.309	-2.425	1.00	84.04	CDK3
ATOM	2041	CA	GLU	362	-5.791	72.002	-2.170	1.00	84.94	CDK3
ATOM	2042	CB	GLU	362	-6.965	71.137	-2.633	1.00	87.42	CDK3
ATOM	2043	CG	GLU	362	-7.480	71.491	-4.027	1.00	92.22	CDK3
ATOM	2044	CD	GLU	362	-8.199	70.335	-4.721	1.00	96.96	CDK3
ATOM	2045	OE1	GLU	362	-8.377	69.261	-4.100	1.00	100.00	CDK3
ATOM	2046	OE2	GLU	362	-8.587	70.505	-5.897	1.00	98.37	CDK3
ATOM	2047	C	GLU	362	-5.942	72.362	-0.695	1.00	85.89	CDK3
ATOM	2048	O	GLU	362	-5.101	71.998	0.122	1.00	84.68	CDK3
ATOM	2049	N	GLU	363	-7.023	73.071	-0.369	1.00	88.39	CDK3
ATOM	2050	CA	GLU	363	-7.302	73.524	0.994	1.00	90.70	CDK3
ATOM	2051	CB	GLU	363	-8.092	74.842	0.944	1.00	94.22	CDK3
ATOM	2052	CG	GLU	363	-7.217	76.108	0.894	1.00	99.19	CDK3
ATOM	2053	CD	GLU	363	-7.806	77.230	0.026	1.00	100.00	CDK3
ATOM	2054	OE1	GLU	363	-7.025	77.924	-0.671	1.00	100.00	CDK3

ATOM	2055	OE2	GLU	363	-9.044	77.421	0.041	1.00	100.00	CDK3
ATOM	2056	C	GLU	363	-8.030	72.524	1.906	1.00	92.38	CDK3
ATOM	2057	O	GLU	363	-7.388	71.865	2.726	1.00	94.13	CDK3
ATOM	2058	N	VAL	364	-9.356	72.424	1.765	1.00	91.55	CDK3
ATOM	2059	CA	VAL	364	-10.219	71.534	2.577	1.00	90.10	CDK3
ATOM	2060	CB	VAL	364	-10.968	70.504	1.702	1.00	90.03	CDK3
ATOM	2061	CG1	VAL	364	-11.956	71.224	0.783	1.00	89.48	CDK3
ATOM	2062	CG2	VAL	364	-9.973	69.664	0.915	1.00	84.62	CDK3
ATOM	2063	C	VAL	364	-9.563	70.767	3.728	1.00	88.07	CDK3
ATOM	2064	O	VAL	364	-8.625	69.999	3.522	1.00	86.37	CDK3
ATOM	2065	N	ASP	365	-10.088	70.960	4.937	1.00	86.95	CDK3
ATOM	2066	CA	ASP	365	-9.535	70.311	6.127	1.00	89.34	CDK3
ATOM	2067	CB	ASP	365	-9.931	71.094	7.390	1.00	89.54	CDK3
ATOM	2068	CG	ASP	365	-11.377	70.865	7.797	1.00	90.95	CDK3
ATOM	2069	OD1	ASP	365	-11.734	71.254	8.931	1.00	88.91	CDK3
ATOM	2070	OD2	ASP	365	-12.152	70.302	6.988	1.00	91.26	CDK3
ATOM	2071	C	ASP	365	-9.952	68.854	6.283	1.00	87.94	CDK3
ATOM	2072	O	ASP	365	-9.338	68.096	7.050	1.00	89.61	CDK3
ATOM	2073	N	PHE	366	-10.985	68.468	5.544	1.00	82.36	CDK3
ATOM	2074	CA	PHE	366	-11.506	67.112	5.608	1.00	77.09	CDK3
ATOM	2075	CB	PHE	366	-10.431	66.079	5.278	1.00	71.64	CDK3
ATOM	2076	CG	PHE	366	-10.936	64.680	5.326	1.00	68.05	CDK3
ATOM	2077	CD1	PHE	366	-10.683	63.875	6.428	1.00	68.33	CDK3
ATOM	2078	CD2	PHE	366	-11.743	64.190	4.306	1.00	66.46	CDK3
ATOM	2079	CE1	PHE	366	-11.237	62.599	6.520	1.00	66.39	CDK3
ATOM	2080	CE2	PHE	366	-12.298	62.921	4.387	1.00	68.12	CDK3
ATOM	2081	CZ	PHE	366	-12.047	62.123	5.498	1.00	65.74	CDK3
ATOM	2082	C	PHE	366	-12.019	66.855	7.011	1.00	74.10	CDK3
ATOM	2083	O	PHE	366	-13.222	66.682	7.215	1.00	72.06	CDK3
ATOM	2084	N	ALA	367	-11.092	66.833	7.969	1.00	71.16	CDK3
ATOM	2085	CA	ALA	367	-11.410	66.610	9.374	1.00	68.61	CDK3
ATOM	2086	CB	ALA	367	-10.267	67.095	10.238	1.00	67.70	CDK3
ATOM	2087	C	ALA	367	-12.699	67.328	9.760	1.00	68.66	CDK3
ATOM	2088	O	ALA	367	-13.495	66.817	10.545	1.00	70.22	CDK3
ATOM	2089	N	GLY	368	-12.901	68.516	9.199	1.00	68.97	CDK3
ATOM	2090	CA	GLY	368	-14.098	69.276	9.498	1.00	67.88	CDK3
ATOM	2091	C	GLY	368	-15.318	68.734	8.781	1.00	69.80	CDK3
ATOM	2092	O	GLY	368	-16.361	68.499	9.401	1.00	70.20	CDK3
ATOM	2093	N	TRP	369	-15.187	68.528	7.472	1.00	69.92	CDK3
ATOM	2094	CA	TRP	369	-16.290	68.012	6.668	1.00	68.55	CDK3
ATOM	2095	CB	TRP	369	-15.851	67.852	5.209	1.00	64.24	CDK3
ATOM	2096	CG	TRP	369	-16.818	67.074	4.406	1.00	64.28	CDK3
ATOM	2097	CD2	TRP	369	-16.840	65.652	4.236	1.00	66.13	CDK3

ATOM	2098	CE2	TRP	369	-17.968	65.345	3.447	1.00	68.08	CDK3
ATOM	2099	CE3	TRP	369	-16.016	64.605	4.675	1.00	63.77	CDK3
ATOM	2100	CD1	TRP	369	-17.896	67.557	3.731	1.00	63.14	CDK3
ATOM	2101	NE1	TRP	369	-18.595	66.528	3.152	1.00	61.49	CDK3
ATOM	2102	CZ2	TRP	369	-18.295	64.029	3.088	1.00	65.55	CDK3
ATOM	2103	CZ3	TRP	369	-16.342	63.299	4.319	1.00	62.74	CDK3
ATOM	2104	CH2	TRP	369	-17.470	63.025	3.534	1.00	64.65	CDK3
ATOM	2105	C	TRP	369	-16.809	66.678	7.211	1.00	68.90	CDK3
ATOM	2106	O	TRP	369	-18.013	66.411	7.168	1.00	68.89	CDK3
ATOM	2107	N	LEU	370	-15.899	65.849	7.721	1.00	66.17	CDK3
ATOM	2108	CA	LEU	370	-16.260	64.548	8.275	1.00	64.64	CDK3
ATOM	2109	CB	LEU	370	-15.012	63.828	8.804	1.00	59.39	CDK3
ATOM	2110	CG	LEU	370	-14.857	62.312	8.653	1.00	52.55	CDK3
ATOM	2111	CD1	LEU	370	-13.704	61.856	9.504	1.00	49.58	CDK3
ATOM	2112	CD2	LEU	370	-16.111	61.592	9.064	1.00	50.86	CDK3
ATOM	2113	C	LEU	370	-17.256	64.738	9.409	1.00	68.06	CDK3
ATOM	2114	O	LEU	370	-18.432	64.409	9.274	1.00	69.83	CDK3
ATOM	2115	N	CYS	371	-16.776	65.282	10.523	1.00	70.84	CDK3
ATOM	2116	CA	CYS	371	-17.613	65.516	11.694	1.00	72.10	CDK3
ATOM	2117	CB	CYS	371	-16.834	66.329	12.712	1.00	73.51	CDK3
ATOM	2118	SG	CYS	371	-15.191	65.648	12.974	1.00	82.20	CDK3
ATOM	2119	C	CYS	371	-18.934	66.197	11.358	1.00	71.16	CDK3
ATOM	2120	O	CYS	371	-19.971	65.871	11.934	1.00	70.42	CDK3
ATOM	2121	N	SER	372	-18.903	67.140	10.428	1.00	70.60	CDK3
ATOM	2122	CA	SER	372	-20.127	67.815	10.024	1.00	72.40	CDK3
ATOM	2123	CB	SER	372	-19.849	68.777	8.872	1.00	73.08	CDK3
ATOM	2124	OG	SER	372	-19.411	70.034	9.346	1.00	75.30	CDK3
ATOM	2125	C	SER	372	-21.119	66.755	9.554	1.00	73.09	CDK3
ATOM	2126	O	SER	372	-22.235	66.662	10.062	1.00	74.85	CDK3
ATOM	2127	N	THR	373	-20.689	65.954	8.584	1.00	72.44	CDK3
ATOM	2128	CA	THR	373	-21.513	64.899	8.007	1.00	70.86	CDK3
ATOM	2129	CB	THR	373	-20.917	64.409	6.676	1.00	69.10	CDK3
ATOM	2130	OG1	THR	373	-20.040	65.407	6.146	1.00	68.71	CDK3
ATOM	2131	CG2	THR	373	-22.015	64.131	5.676	1.00	66.50	CDK3
ATOM	2132	C	THR	373	-21.676	63.692	8.927	1.00	72.35	CDK3
ATOM	2133	O	THR	373	-22.792	63.257	9.203	1.00	69.68	CDK3
ATOM	2134	N	ILE	374	-20.556	63.143	9.383	1.00	76.62	CDK3
ATOM	2135	CA	ILE	374	-20.560	61.981	10.270	1.00	79.38	CDK3
ATOM	2136	CB	ILE	374	-19.116	61.479	10.517	1.00	77.35	CDK3
ATOM	2137	CG2	ILE	374	-18.343	62.504	11.311	1.00	80.65	CDK3
ATOM	2138	CG1	ILE	374	-19.123	60.175	11.302	1.00	73.92	CDK3
ATOM	2139	CD1	ILE	374	-17.737	59.729	11.726	1.00	72.50	CDK3
ATOM	2140	C	ILE	374	-21.202	62.336	11.610	1.00	83.05	CDK3

ATOM	2141	O	ILE	374	-21.590	61.458	12.378	1.00 85.50	CDK3
ATOM	2142	N	GLY	375	-21.314	63.633	11.883	1.00 85.38	CDK3
ATOM	2143	CA	GLY	375	-21.904	64.075	13.130	1.00 84.58	CDK3
ATOM	2144	C	GLY	375	-20.966	63.883	14.305	1.00 86.76	CDK3
ATOM	2145	O	GLY	375	-21.362	63.356	15.340	1.00 84.45	CDK3
ATOM	2146	N	LEU	376	-19.715	64.302	14.148	1.00 89.97	CDK3
ATOM	2147	CA	LEU	376	-18.729	64.175	15.216	1.00 92.83	CDK3
ATOM	2148	CB	LEU	376	-17.408	63.642	14.655	1.00 93.90	CDK3
ATOM	2149	CG	LEU	376	-17.242	62.119	14.614	1.00 93.66	CDK3
ATOM	2150	CD1	LEU	376	-15.982	61.762	13.836	1.00 93.31	CDK3
ATOM	2151	CD2	LEU	376	-17.174	61.568	16.032	1.00 91.79	CDK3
ATOM	2152	C	LEU	376	-18.512	65.537	15.873	1.00 95.46	CDK3
ATOM	2153	O	LEU	376	-17.540	65.747	16.604	1.00 94.72	CDK3
ATOM	2154	N	ALA	377	-19.435	66.457	15.603	1.00 98.71	CDK3
ATOM	2155	CA	ALA	377	-19.383	67.810	16.150	1.00 99.99	CDK3
ATOM	2156	CB	ALA	377	-19.210	68.827	15.013	1.00 99.14	CDK3
ATOM	2157	C	ALA	377	-20.653	68.118	16.952	1.00100.00	CDK3
ATOM	2158	O	ALA	377	-21.243	67.168	17.516	1.00 98.40	CDK3
ATOM	2159	OT	ALA	377	-21.040	69.308	17.008	1.00100.00	CDK3
ATOM	2160	C1	318	1	-6.500	44.841	10.293	1.00 41.59	INH_
ATOM	2161	C2	318	1	-7.148	43.585	9.859	1.00 36.80	INH_
ATOM	2162	C3	318	1	-6.541	42.782	8.781	1.00 40.22	INH_
ATOM	2163	C4	318	1	-5.251	43.279	8.147	1.00 32.59	INH_
ATOM	2164	C5	318	1	-4.628	44.463	8.552	1.00 40.44	INH_
ATOM	2165	C6	318	1	-5.256	45.242	9.628	1.00 39.82	INH_
ATOM	2166	I1	318	1	-4.302	46.888	10.123	1.00 44.61	INH_
ATOM	2167	C8	318	1	-8.091	40.202	6.520	1.00 45.14	INH_
ATOM	2168	C9	318	1	-7.824	39.225	5.473	1.00 35.85	INH_
ATOM	2169	C10	318	1	-6.475	38.655	5.329	1.00 38.09	INH_
ATOM	2170	C11	318	1	-5.379	39.052	6.234	1.00 40.23	INH_
ATOM	2171	C12	318	1	-5.635	39.986	7.238	1.00 39.98	INH_
ATOM	2172	C13	318	1	-6.965	40.608	7.430	1.00 39.86	INH_
ATOM	2173	CL1	318	1	-6.247	37.438	3.974	1.00 29.67	INH_
ATOM	2174	F1	318	1	-4.113	38.558	6.151	1.00 48.51	INH_
ATOM	2175	F2	318	1	-4.640	40.297	8.001	1.00 43.48	INH_
ATOM	2176	F3	318	1	-8.265	43.239	10.476	1.00 51.02	INH_
ATOM	2177	N1	318	1	-7.236	41.564	8.418	1.00 37.83	INH_
ATOM	2178	C7	318	1	-9.458	40.776	6.669	1.00 50.44	INH_
ATOM	2179	O1	318	1	-9.709	41.591	7.543	1.00 55.21	INH_
ATOM	2180	N2	318	1	-10.427	40.367	5.815	1.00 52.60	INH_
ATOM	2181	O2	318	1	-11.804	41.104	6.159	1.00 69.87	INH_
ATOM	2182	O3	318	1	-16.065	40.590	7.270	1.00 75.43	INH_
ATOM	2183	O4	318	1	-13.623	40.219	8.431	1.00 70.02	INH_

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ATOM   2184  C14 318     1     -12.954  40.092   5.887  1.00 66.96      INH_
ATOM   2185  C15 318     1     -13.808  39.712   7.103  1.00 70.71      INH_
ATOM   2186  C16 318     1     -15.159  39.895   6.401  1.00 72.65      INH_
ATOM   2187  O3G ATP   400     -15.568  42.181   3.829  1.00 44.15      ATP_
ATOM   2188  PG  ATP   400     -17.053  42.591   3.985  1.00 44.92      ATP_
ATOM   2189  O1G ATP   400     -17.892  41.366   4.366  1.00 58.57      ATP_
ATOM   2190  O2G ATP   400     -17.637  43.187   2.678  1.00 61.48      ATP_
ATOM   2191  O3B ATP   400     -17.217  43.571   5.141  1.00 49.44      ATP_
ATOM   2192  PB  ATP   400     -16.565  44.698   6.001  1.00 38.78      ATP_
ATOM   2193  O1B ATP   400     -15.135  45.272   5.763  1.00 31.80      ATP_
ATOM   2194  O2B ATP   400     -17.591  45.846   6.010  1.00 22.91      ATP_
ATOM   2195  O3A ATP   400     -16.451  44.136   7.380  1.00 39.48      ATP_
ATOM   2196  PA  ATP   400     -15.455  43.881   8.477  1.00 41.79      ATP_
ATOM   2197  O1A ATP   400     -15.932  42.594   9.200  1.00 43.90      ATP_
ATOM   2198  O2A ATP   400     -13.936  43.715   8.096  1.00 49.00      ATP_
ATOM   2199  O5* ATP   400     -15.612  45.251   9.228  1.00 36.00      ATP_
ATOM   2200  C5* ATP   400     -16.999  45.650   9.506  1.00 38.86      ATP_
ATOM   2201  C4* ATP   400     -17.268  47.152   9.700  1.00 47.98      ATP_
ATOM   2202  C3* ATP   400     -16.671  48.206   8.721  1.00 46.21      ATP_
ATOM   2203  C2* ATP   400     -16.420  49.399   9.676  1.00 44.34      ATP_
ATOM   2204  C1* ATP   400     -16.159  48.732  11.025  1.00 40.50      ATP_
ATOM   2205  O4* ATP   400     -16.894  47.516  11.044  1.00 46.25      ATP_
ATOM   2206  C4  ATP   400     -14.040  49.644  12.235  1.00 33.84      ATP_
ATOM   2207  N9  ATP   400     -14.731  48.699  11.449  1.00 31.46      ATP_
ATOM   2208  C8  ATP   400     -13.870  47.689  11.110  1.00 23.90      ATP_
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ATOM   2210  C5  ATP   400     -12.725  49.143  12.340  1.00 24.46      ATP_
ATOM   2211  C2  ATP   400     -13.505  51.536  13.539  1.00 29.27      ATP_
ATOM   2212  N3  ATP   400     -14.444  50.856  12.839  1.00 32.24      ATP_
ATOM   2213  C6  ATP   400     -11.840  49.910  13.073  1.00 30.06      ATP_
ATOM   2214  N1  ATP   400     -12.236  51.090  13.661  1.00 26.42      ATP_
ATOM   2215  O2* ATP   400     -17.628  50.185   9.792  1.00 48.68      ATP_
ATOM   2216  O3* ATP   400     -17.638  48.686   7.748  1.00 51.62      ATP_
ATOM   2217  N6  ATP   400     -10.544  49.505  13.220  1.00 22.69      ATP_
ATOM   2218  MG2 MG2   500     -13.179  45.151   6.491  1.00 37.75      MG__
ATOM   2219  OH2 TIP3  601       3.025  37.344   6.739  1.00 53.17      W___
ATOM   2220  OH2 TIP3  602     -13.683  43.453   4.857  1.00 34.52      W___
ATOM   2221  OH2 TIP3  603       0.029  51.965  10.856  1.00 39.17      W___
ATOM   2222  OH2 TIP3  604     -11.555  46.113   9.597  1.00 37.07      W___
ATOM   2223  OH2 TIP3  605      -3.444  42.053  27.061  1.00 47.09      W___
ATOM   2224  OH2 TIP3  606       8.199  50.693   8.139  1.00 73.41      W___
ATOM   2225  OH2 TIP3  607     -25.760  57.484  -0.801  1.00 65.11      W___
ATOM   2226  OH2 TIP3  608      -0.365  50.730  16.444  1.00 48.92      W___
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ATOM	2227	OH2	TIP3	609	1.924	47.459	16.182	1.00	61.85	W
ATOM	2228	OH2	TIP3	610	3.756	61.475	3.241	1.00	68.67	W
ATOM	2229	OH2	TIP3	611	-8.237	45.166	-4.274	1.00	40.78	W
ATOM	2230	OH2	TIP3	612	4.049	54.701	-6.071	1.00	44.38	W
ATOM	2231	OH2	TIP3	613	-17.770	48.776	0.444	1.00	52.53	W
ATOM	2232	OH2	TIP3	614	-9.547	43.756	-7.764	1.00	40.97	W
ATOM	2233	OH2	TIP3	615	-10.853	56.267	20.980	1.00	71.55	W
ATOM	2234	OH2	TIP3	616	-13.421	56.230	22.695	1.00	68.64	W
ATOM	2235	OH2	TIP3	617	-9.657	67.634	-5.721	1.00	57.63	W
ATOM	2236	OH2	TIP3	618	3.439	41.911	-4.619	1.00	43.43	W
ATOM	2237	OH2	TIP3	619	-24.225	63.324	-10.630	1.00	62.89	W
ATOM	2238	OH2	TIP3	620	-15.557	70.845	-10.249	1.00	60.89	W
ATOM	2239	OH2	TIP3	621	0.534	37.266	1.709	1.00	44.51	W
ATOM	2240	OH2	TIP3	622	-6.632	52.860	18.986	1.00	28.55	W
ATOM	2241	OH2	TIP3	623	-4.050	59.469	6.428	1.00	42.86	W
ATOM	2242	OH2	TIP3	624	-19.724	63.593	-5.680	1.00	65.70	W
ATOM	2243	OH2	TIP3	625	-11.123	35.564	19.665	1.00	61.26	W
ATOM	2244	OH2	TIP3	626	3.587	55.888	0.634	1.00	41.35	W
ATOM	2245	OH2	TIP3	627	0.067	38.213	-6.671	1.00	56.60	W
ATOM	2246	OH2	TIP3	628	-11.916	41.396	-20.060	1.00	62.25	W
ATOM	2247	OH2	TIP3	629	-16.623	46.898	-16.807	1.00	52.26	W
ATOM	2248	OH2	TIP3	630	2.880	37.359	1.906	1.00	52.99	W
ATOM	2249	OH2	TIP3	631	-14.180	70.642	-7.649	1.00	64.98	W
ATOM	2250	OH2	TIP3	632	-17.316	51.891	12.735	1.00	41.22	W
ATOM	2251	OH2	TIP3	633	-20.586	59.455	14.363	1.00	62.98	W
ATOM	2252	OH2	TIP3	634	-16.171	72.773	-8.183	1.00	79.27	W
ATOM	2253	OH2	TIP3	635	-1.030	32.622	-11.872	1.00	71.42	W
ATOM	2254	OH2	TIP3	636	-32.155	40.676	-13.246	1.00	55.63	W
ATOM	2255	OH2	TIP3	637	-5.106	56.011	-20.714	1.00	43.06	W
ATOM	2256	OH2	TIP3	638	-3.311	26.862	19.215	1.00	75.69	W
ATOM	2257	OH2	TIP3	639	-4.723	60.999	-21.970	1.00	89.78	W
ATOM	2258	OH2	TIP3	640	-0.377	39.847	21.273	1.00	52.42	W
ATOM	2259	OH2	TIP3	641	-12.209	52.786	27.788	1.00	64.87	W
ATOM	2260	OH2	TIP3	642	1.993	35.335	4.568	1.00	76.31	W
ATOM	2261	OH2	TIP3	643	-9.760	42.230	-5.069	1.00	49.26	W
ATOM	2262	OH2	TIP3	644	9.035	51.460	11.840	1.00	61.28	W
ATOM	2263	OH2	TIP3	645	-18.773	48.711	-26.779	1.00	64.38	W
ATOM	2264	OH2	TIP3	646	-17.321	53.047	-19.961	1.00	52.72	W
ATOM	2265	OH2	TIP3	647	0.455	35.903	19.143	1.00	50.49	W
ATOM	2266	OH2	TIP3	648	-15.950	50.772	29.139	1.00	58.49	W
ATOM	2267	OH2	TIP3	649	-13.391	47.071	7.553	1.00	43.80	W
ATOM	2268	OH2	TIP3	650	-16.832	67.979	-8.019	1.00	76.40	W
ATOM	2269	OH2	TIP3	651	-20.162	55.718	11.696	1.00	81.21	W

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ATOM   2270  OH2 TIP3  652      -2.070  53.141  31.048  1.00 36.42      W___
ATOM   2271  OH2 TIP3  653     -15.438  42.458  -4.017  1.00 24.54      W___
ATOM   2272  OH2 TIP3  654     -15.505  45.102  -9.920  1.00 30.66      W___
ATOM   2273  OH2 TIP3  655     -23.593  52.736  -2.584  1.00 50.00      W___
ATOM   2274  OH2 TIP3  656     -16.328  40.130  -3.901  1.00 45.83      W___
ATOM   2275  OH2 TIP3  657      -9.692  57.673  15.853  1.00 55.14      W___
ATOM   2276  OH2 TIP3  658     -16.420  39.179  -6.536  1.00 48.09      W___
ATOM   2277  OH2 TIP3  659       1.502  40.580  -5.444  1.00 43.26      W___
ATOM   2278  OH2 TIP3  660     -26.007  51.379  -3.652  1.00 53.45      W___
ATOM   2279  OH2 TIP3  661      -5.859  67.920  -0.057  1.00 52.36      W___
ATOM   2280  OH2 TIP3  662      -7.502  56.436  15.491  1.00 33.61      W___
ATOM   2281  OH2 TIP3  663      -1.321  40.428  -0.223  1.00 46.80      W___
ATOM   2282  OH2 TIP3  664      -7.584  55.239  18.429  1.00 43.98      W___
ATOM   2283  OH2 TIP3  665     -21.246  50.532 -18.236  1.00 56.71      W___
ATOM   2284  OH2 TIP3  666     -22.943  66.872   4.384  1.00 70.38      W___
ATOM   2285  OH2 TIP3  667       0.334  39.519  28.390  1.00 56.47      W___
ATOM   2286  OH2 TIP3  668     -17.809  45.837   2.074  1.00 59.28      W___
ATOM   2287  OH2 TIP3  669     -25.765  65.209 -10.517  1.00 67.23      W___
ATOM   2288  OH2 TIP3  670     -17.027  36.269 -21.031  1.00 47.08      W___
ATOM   2289  OH2 TIP3  671      -1.660  31.898  -0.229  1.00 48.35      W___
ATOM   2290  OH2 TIP3  672      -0.621  58.566  11.653  1.00 75.01      W___
ATOM   2291  OH2 TIP3  673     -30.112  55.477 -10.246  1.00 77.58      W___
ATOM   2292  OH2 TIP3  674     -21.608  69.267   6.492  1.00 87.08      W___
ATOM   2293  OH2 TIP3  675     -20.130  51.711  -0.208  1.00 48.81      W___
ATOM   2294  OH2 TIP3  676     -14.303  40.664  22.090  1.00 76.34      W___
ATOM   2295  OH2 TIP3  677      -0.457  49.839  -8.994  1.00 77.62      W___
ATOM   2296  OH2 TIP3  678     -33.589  56.072 -14.198  1.00100.00      W___
ATOM   2297  OH2 TIP3  679       0.880  48.786  13.638  1.00 50.42      W___
ATOM   2298  OH2 TIP3  680       5.938  50.884  15.016  1.00 65.16      W___
END
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Table 2
Crystal Coordinates of the MEK2: MgATP: {5-[3,4-Difluoro-2-(2-fluoro-4-iodo-phenylamino)-phenyl]-1,3,4-oxadiazol-2-yl}-(2-morpholin-4-yl-ethyl)-amine Ternary Complex

ATOM	1	CB	ALA	A	62	24.914	145.101	16.487	1.00	49.09	A	C
ATOM	2	C	ALA	A	62	24.557	142.674	15.866	1.00	60.39	A	C
ATOM	3	O	ALA	A	62	24.249	142.030	16.882	1.00	60.85	A	O
ATOM	4	N	ALA	A	62	22.639	144.240	16.031	1.00	60.72	A	N
ATOM	5	CA	ALA	A	62	24.076	144.117	15.661	1.00	60.38	A	C
ATOM	6	N	LYS	A	63	25.312	142.181	14.882	1.00	103.30	A	N
ATOM	7	CA	LYS	A	63	25.833	140.812	14.869	1.00	105.41	A	C
ATOM	8	CB	LYS	A	63	25.447	140.130	13.549	1.00	65.41	A	C
ATOM	9	CG	LYS	A	63	24.017	140.436	13.049	1.00	65.48	A	C
ATOM	10	CD	LYS	A	63	22.891	139.693	13.811	1.00	65.65	A	C
ATOM	11	CE	LYS	A	63	22.642	140.221	15.223	1.00	65.41	A	C
ATOM	12	NZ	LYS	A	63	22.023	141.573	15.259	1.00	65.35	A	N
ATOM	13	C	LYS	A	63	27.350	140.735	15.033	1.00	106.31	A	C
ATOM	14	O	LYS	A	63	28.042	140.197	14.171	1.00	106.08	A	O
ATOM	15	N	VAL	A	64	27.859	141.258	16.143	1.00	78.44	A	N
ATOM	16	CA	VAL	A	64	29.291	141.248	16.407	1.00	77.77	A	C
ATOM	17	CB	VAL	A	64	29.636	142.225	17.534	1.00	46.45	A	C
ATOM	18	CG1	VAL	A	64	28.367	142.948	17.985	1.00	46.43	A	C
ATOM	19	CG2	VAL	A	64	30.307	141.482	18.695	1.00	47.47	A	C
ATOM	20	C	VAL	A	64	29.811	139.867	16.790	1.00	78.33	A	C
ATOM	21	O	VAL	A	64	29.184	139.154	17.581	1.00	78.22	A	O
ATOM	22	N	GLY	A	65	30.965	139.501	16.229	1.00	87.05	A	N
ATOM	23	CA	GLY	A	65	31.565	138.208	16.517	1.00	86.59	A	C
ATOM	24	C	GLY	A	65	33.023	138.289	16.941	1.00	85.82	A	C
ATOM	25	O	GLY	A	65	33.896	138.568	16.115	1.00	85.51	A	O
ATOM	26	N	GLU	A	66	33.278	138.040	18.227	1.00	196.62	A	N
ATOM	27	CA	GLU	A	66	34.629	138.069	18.801	1.00	196.16	A	C
ATOM	28	CB	GLU	A	66	34.817	139.330	19.653	1.00	95.24	A	C
ATOM	29	CG	GLU	A	66	36.005	139.275	20.615	1.00	96.53	A	C
ATOM	30	CD	GLU	A	66	35.579	139.326	22.077	1.00	98.06	A	C
ATOM	31	OE1	GLU	A	66	36.461	139.313	22.959	1.00	98.88	A	O
ATOM	32	OE2	GLU	A	66	34.361	139.382	22.347	1.00	98.60	A	O
ATOM	33	C	GLU	A	66	34.902	136.839	19.668	1.00	195.80	A	C
ATOM	34	O	GLU	A	66	34.601	136.839	20.862	1.00	194.35	A	O
ATOM	35	N	LEU	A	67	35.479	135.796	19.074	1.00	72.53	A	N
ATOM	36	CA	LEU	A	67	35.769	134.578	19.828	1.00	71.13	A	C
ATOM	37	CB	LEU	A	67	34.481	134.025	20.448	1.00	110.03	A	C

ATOM	38	CG	LEU	A	67	33.497	133.378	19.467	1.00107.97	A	C
ATOM	39	CD1	LEU	A	67	33.381	131.888	19.789	1.00107.39	A	C
ATOM	40	CD2	LEU	A	67	32.133	134.069	19.547	1.00105.11	A	C
ATOM	41	C	LEU	A	67	36.427	133.471	19.010	1.00 71.78	A	C
ATOM	42	O	LEU	A	67	36.430	133.515	17.780	1.00 71.36	A	O
ATOM	43	N	LYS	A	68	36.982	132.489	19.725	1.00157.42	A	N
ATOM	44	CA	LYS	A	68	37.643	131.313	19.145	1.00156.89	A	C
ATOM	45	CB	LYS	A	68	39.036	131.661	18.594	1.00150.17	A	C
ATOM	46	CG	LYS	A	68	39.721	130.515	17.821	1.00151.06	A	C
ATOM	47	CD	LYS	A	68	38.896	130.067	16.610	1.00152.37	A	C
ATOM	48	CE	LYS	A	68	39.503	128.856	15.897	1.00151.85	A	C
ATOM	49	NZ	LYS	A	68	40.811	129.146	15.245	1.00150.48	A	N
ATOM	50	C	LYS	A	68	37.767	130.239	20.229	1.00156.18	A	C
ATOM	51	O	LYS	A	68	36.769	129.876	20.852	1.00155.87	A	O
ATOM	52	N	ASP	A	69	38.979	129.741	20.472	1.00 91.56	A	N
ATOM	53	CA	ASP	A	69	39.156	128.698	21.484	1.00 91.07	A	C
ATOM	54	CB	ASP	A	69	38.426	127.435	21.036	1.00146.37	A	C
ATOM	55	CG	ASP	A	69	38.742	127.067	19.603	1.00146.93	A	C
ATOM	56	OD1	ASP	A	69	38.209	127.732	18.689	1.00149.03	A	O
ATOM	57	OD2	ASP	A	69	39.533	126.125	19.391	1.00146.17	A	O
ATOM	58	C	ASP	A	69	40.594	128.321	21.843	1.00 89.27	A	C
ATOM	59	O	ASP	A	69	41.241	127.572	21.114	1.00 88.69	A	O
ATOM	60	N	ASP	A	70	41.071	128.813	22.983	1.00102.16	A	N
ATOM	61	CA	ASP	A	70	42.423	128.517	23.448	1.00101.34	A	C
ATOM	62	CB	ASP	A	70	43.426	128.602	22.295	1.00109.37	A	C
ATOM	63	CG	ASP	A	70	44.868	128.510	22.769	1.00110.03	A	C
ATOM	64	OD1	ASP	A	70	45.312	129.405	23.525	1.00109.11	A	O
ATOM	65	OD2	ASP	A	70	45.557	127.539	22.385	1.00112.08	A	O
ATOM	66	C	ASP	A	70	42.870	129.473	24.539	1.00100.17	A	C
ATOM	67	O	ASP	A	70	43.468	129.070	25.540	1.00100.21	A	O
ATOM	68	N	ASP	A	71	42.595	130.751	24.324	1.00111.53	A	N
ATOM	69	CA	ASP	A	71	42.980	131.780	25.271	1.00110.44	A	C
ATOM	70	CB	ASP	A	71	42.667	133.150	24.679	1.00136.33	A	C
ATOM	71	CG	ASP	A	71	43.431	133.418	23.392	1.00135.16	A	C
ATOM	72	OD1	ASP	A	71	44.662	133.628	23.457	1.00134.65	A	O
ATOM	73	OD2	ASP	A	71	42.797	133.413	22.314	1.00134.71	A	O
ATOM	74	C	ASP	A	71	42.277	131.613	26.611	1.00109.38	A	C
ATOM	75	O	ASP	A	71	41.526	132.484	27.031	1.00108.12	A	O
ATOM	76	N	PHE	A	72	42.517	130.482	27.271	1.00 92.50	A	N
ATOM	77	CA	PHE	A	72	41.919	130.203	28.572	1.00 90.40	A	C
ATOM	78	CB	PHE	A	72	40.645	129.355	28.453	1.00 46.35	A	C
ATOM	79	CG	PHE	A	72	39.710	129.792	27.374	1.00 43.59	A	C
ATOM	80	CD1	PHE	A	72	39.976	129.487	26.052	1.00 41.55	A	C

ATOM	81	CD2	PHE	A	72	38.549	130.469	27.683	1.00	42.18	A	C
ATOM	82	CE1	PHE	A	72	39.103	129.843	25.066	1.00	40.19	A	C
ATOM	83	CE2	PHE	A	72	37.671	130.829	26.701	1.00	41.57	A	C
ATOM	84	CZ	PHE	A	72	37.944	130.515	25.390	1.00	40.24	A	C
ATOM	85	C	PHE	A	72	42.894	129.419	29.432	1.00	90.64	A	C
ATOM	86	O	PHE	A	72	43.212	128.270	29.120	1.00	89.73	A	O
ATOM	87	N	GLU	A	73	43.361	130.029	30.516	1.00	68.60	A	N
ATOM	88	CA	GLU	A	73	44.275	129.348	31.425	1.00	69.96	A	C
ATOM	89	CB	GLU	A	73	45.329	130.313	31.974	1.00	159.16	A	C
ATOM	90	CG	GLU	A	73	46.237	130.926	30.929	1.00	161.01	A	C
ATOM	91	CD	GLU	A	73	46.865	129.888	30.024	1.00	162.55	A	C
ATOM	92	OE1	GLU	A	73	47.331	128.850	30.543	1.00	163.42	A	O
ATOM	93	OE2	GLU	A	73	46.899	130.114	28.795	1.00	164.96	A	O
ATOM	94	C	GLU	A	73	43.479	128.787	32.593	1.00	71.43	A	C
ATOM	95	O	GLU	A	73	42.949	129.547	33.395	1.00	71.30	A	O
ATOM	96	N	ARG	A	74	43.369	127.467	32.677	1.00	62.36	A	N
ATOM	97	CA	ARG	A	74	42.650	126.871	33.788	1.00	63.19	A	C
ATOM	98	CB	ARG	A	74	42.984	125.383	33.927	1.00	140.82	A	C
ATOM	99	CG	ARG	A	74	42.120	124.433	33.123	1.00	141.51	A	C
ATOM	100	CD	ARG	A	74	42.645	123.012	33.268	1.00	139.81	A	C
ATOM	101	NE	ARG	A	74	43.935	122.849	32.597	1.00	139.25	A	N
ATOM	102	CZ	ARG	A	74	44.078	122.618	31.294	1.00	138.86	A	C
ATOM	103	NH1	ARG	A	74	43.011	122.514	30.512	1.00	138.88	A	N
ATOM	104	NH2	ARG	A	74	45.289	122.498	30.769	1.00	138.63	A	N
ATOM	105	C	ARG	A	74	43.155	127.597	35.023	1.00	63.52	A	C
ATOM	106	O	ARG	A	74	44.195	127.245	35.564	1.00	63.01	A	O
ATOM	107	N	ILE	A	75	42.441	128.623	35.460	1.00	67.77	A	N
ATOM	108	CA	ILE	A	75	42.865	129.362	36.638	1.00	69.65	A	C
ATOM	109	CB	ILE	A	75	42.413	130.842	36.558	1.00	91.85	A	C
ATOM	110	CG2	ILE	A	75	41.313	130.990	35.531	1.00	93.51	A	C
ATOM	111	CG1	ILE	A	75	41.957	131.342	37.930	1.00	92.07	A	C
ATOM	112	CD1	ILE	A	75	41.585	132.812	37.950	1.00	92.80	A	C
ATOM	113	C	ILE	A	75	42.300	128.697	37.887	1.00	69.80	A	C
ATOM	114	O	ILE	A	75	42.787	128.913	38.998	1.00	69.14	A	O
ATOM	115	N	SER	A	76	41.283	127.864	37.689	1.00	94.92	A	N
ATOM	116	CA	SER	A	76	40.641	127.148	38.786	1.00	95.75	A	C
ATOM	117	CB	SER	A	76	39.989	128.128	39.771	1.00	107.49	A	C
ATOM	118	OG	SER	A	76	40.940	128.972	40.397	1.00	107.47	A	O
ATOM	119	C	SER	A	76	39.567	126.209	38.253	1.00	95.64	A	C
ATOM	120	O	SER	A	76	39.193	126.264	37.083	1.00	97.35	A	O
ATOM	121	N	GLU	A	77	39.076	125.343	39.127	1.00	96.80	A	N
ATOM	122	CA	GLU	A	77	38.025	124.410	38.765	1.00	95.51	A	C
ATOM	123	CB	GLU	A	77	38.532	122.973	38.912	1.00	50.29	A	C

ATOM	124	CG	GLU	A	77	39.385	122.498	37.735	1.00	49.05	A	C
ATOM	125	CD	GLU	A	77	38.548	121.952	36.577	1.00	48.46	A	C
ATOM	126	OE1	GLU	A	77	39.078	121.842	35.453	1.00	49.14	A	O
ATOM	127	OE2	GLU	A	77	37.365	121.615	36.789	1.00	46.77	A	O
ATOM	128	C	GLU	A	77	36.869	124.701	39.712	1.00	96.22	A	C
ATOM	129	O	GLU	A	77	37.032	124.664	40.930	1.00	96.70	A	O
ATOM	130	N	LEU	A	78	35.706	125.011	39.148	1.00	103.61	A	N
ATOM	131	CA	LEU	A	78	34.538	125.353	39.951	1.00	105.65	A	C
ATOM	132	CB	LEU	A	78	33.616	126.272	39.147	1.00	45.76	A	C
ATOM	133	CG	LEU	A	78	34.289	127.517	38.570	1.00	45.20	A	C
ATOM	134	CD1	LEU	A	78	33.269	128.393	37.881	1.00	43.93	A	C
ATOM	135	CD2	LEU	A	78	34.972	128.280	39.686	1.00	44.41	A	C
ATOM	136	C	LEU	A	78	33.742	124.159	40.467	1.00	106.69	A	C
ATOM	137	O	LEU	A	78	33.685	123.916	41.678	1.00	106.47	A	O
ATOM	138	N	GLY	A	79	33.118	123.426	39.548	1.00	44.50	A	N
ATOM	139	CA	GLY	A	79	32.329	122.273	39.937	1.00	46.32	A	C
ATOM	140	C	GLY	A	79	32.029	121.362	38.768	1.00	47.26	A	C
ATOM	141	O	GLY	A	79	32.739	121.376	37.763	1.00	48.04	A	O
ATOM	142	N	ALA	A	80	30.974	120.567	38.905	1.00	77.76	A	N
ATOM	143	CA	ALA	A	80	30.569	119.639	37.861	1.00	76.70	A	C
ATOM	144	CB	ALA	A	80	31.717	118.701	37.515	1.00	29.17	A	C
ATOM	145	C	ALA	A	80	29.356	118.822	38.283	1.00	77.52	A	C
ATOM	146	O	ALA	A	80	29.236	118.406	39.435	1.00	78.22	A	O
ATOM	147	N	GLY	A	81	28.458	118.597	37.333	1.00	76.59	A	N
ATOM	148	CA	GLY	A	81	27.271	117.813	37.592	1.00	77.33	A	C
ATOM	149	C	GLY	A	81	27.093	116.865	36.427	1.00	77.54	A	C
ATOM	150	O	GLY	A	81	28.075	116.374	35.864	1.00	77.93	A	O
ATOM	151	N	ASN	A	82	25.845	116.600	36.061	1.00	78.30	A	N
ATOM	152	CA	ASN	A	82	25.571	115.722	34.937	1.00	80.35	A	C
ATOM	153	CB	ASN	A	82	24.470	114.719	35.293	1.00	192.95	A	C
ATOM	154	CG	ASN	A	82	25.011	113.496	36.010	1.00	194.40	A	C
ATOM	155	OD1	ASN	A	82	25.853	112.774	35.473	1.00	194.61	A	O
ATOM	156	ND2	ASN	A	82	24.530	113.257	37.225	1.00	195.32	A	N
ATOM	157	C	ASN	A	82	25.161	116.563	33.740	1.00	80.83	A	C
ATOM	158	O	ASN	A	82	24.217	117.346	33.813	1.00	81.51	A	O
ATOM	159	N	GLY	A	83	25.888	116.397	32.641	1.00	113.81	A	N
ATOM	160	CA	GLY	A	83	25.607	117.151	31.436	1.00	112.43	A	C
ATOM	161	C	GLY	A	83	26.845	117.904	30.991	1.00	111.16	A	C
ATOM	162	O	GLY	A	83	26.958	118.311	29.837	1.00	111.08	A	O
ATOM	163	N	GLY	A	84	27.781	118.089	31.916	1.00	74.91	A	N
ATOM	164	CA	GLY	A	84	29.004	118.796	31.594	1.00	72.12	A	C
ATOM	165	C	GLY	A	84	29.967	118.874	32.761	1.00	70.95	A	C
ATOM	166	O	GLY	A	84	30.248	117.878	33.419	1.00	71.32	A	O

ATOM	167	N	VAL	A	85	30.473	120.075	33.008	1.00	49.49	A	N
ATOM	168	CA	VAL	A	85	31.419	120.350	34.083	1.00	48.80	A	C
ATOM	169	CB	VAL	A	85	32.512	119.274	34.183	1.00	38.40	A	C
ATOM	170	CG1	VAL	A	85	33.086	118.955	32.794	1.00	38.94	A	C
ATOM	171	CG2	VAL	A	85	33.599	119.754	35.130	1.00	38.78	A	C
ATOM	172	C	VAL	A	85	32.048	121.699	33.755	1.00	47.13	A	C
ATOM	173	O	VAL	A	85	32.489	121.922	32.629	1.00	45.92	A	O
ATOM	174	N	VAL	A	86	32.093	122.589	34.742	1.00	41.32	A	N
ATOM	175	CA	VAL	A	86	32.593	123.947	34.534	1.00	40.22	A	C
ATOM	176	CB	VAL	A	86	31.452	124.972	34.785	1.00	51.28	A	C
ATOM	177	CG1	VAL	A	86	30.397	124.366	35.686	1.00	52.20	A	C
ATOM	178	CG2	VAL	A	86	32.008	126.227	35.433	1.00	52.04	A	C
ATOM	179	C	VAL	A	86	33.815	124.388	35.317	1.00	38.65	A	C
ATOM	180	O	VAL	A	86	33.878	124.259	36.536	1.00	38.37	A	O
ATOM	181	N	THR	A	87	34.777	124.951	34.602	1.00	73.63	A	N
ATOM	182	CA	THR	A	87	36.010	125.414	35.219	1.00	73.38	A	C
ATOM	183	CB	THR	A	87	37.213	124.650	34.642	1.00	58.83	A	C
ATOM	184	OG1	THR	A	87	38.379	125.478	34.696	1.00	59.67	A	O
ATOM	185	CG2	THR	A	87	36.944	124.256	33.206	1.00	57.85	A	C
ATOM	186	C	THR	A	87	36.238	126.905	35.005	1.00	73.60	A	C
ATOM	187	O	THR	A	87	36.018	127.415	33.904	1.00	74.23	A	O
ATOM	188	N	LYS	A	88	36.668	127.609	36.054	1.00	63.79	A	N
ATOM	189	CA	LYS	A	88	36.939	129.040	35.915	1.00	63.61	A	C
ATOM	190	CB	LYS	A	88	37.112	129.755	37.260	1.00	36.81	A	C
ATOM	191	CG	LYS	A	88	37.365	131.256	37.075	1.00	38.64	A	C
ATOM	192	CD	LYS	A	88	37.990	131.936	38.298	1.00	39.59	A	C
ATOM	193	CE	LYS	A	88	37.030	132.063	39.473	1.00	40.95	A	C
ATOM	194	NZ	LYS	A	88	37.563	132.965	40.537	1.00	41.07	A	N
ATOM	195	C	LYS	A	88	38.231	129.178	35.143	1.00	64.41	A	C
ATOM	196	O	LYS	A	88	39.305	128.858	35.643	1.00	62.13	A	O
ATOM	197	N	VAL	A	89	38.113	129.649	33.915	1.00	75.08	A	N
ATOM	198	CA	VAL	A	89	39.265	129.836	33.067	1.00	75.12	A	C
ATOM	199	CB	VAL	A	89	39.077	129.079	31.754	1.00	48.39	A	C
ATOM	200	CG1	VAL	A	89	38.853	127.611	32.041	1.00	50.04	A	C
ATOM	201	CG2	VAL	A	89	37.893	129.634	31.008	1.00	47.84	A	C
ATOM	202	C	VAL	A	89	39.364	131.326	32.789	1.00	75.38	A	C
ATOM	203	O	VAL	A	89	38.405	132.062	33.017	1.00	74.93	A	O
ATOM	204	N	GLN	A	90	40.523	131.782	32.324	1.00	63.94	A	N
ATOM	205	CA	GLN	A	90	40.676	133.194	32.005	1.00	65.40	A	C
ATOM	206	CB	GLN	A	90	41.754	133.848	32.859	1.00	103.39	A	C
ATOM	207	CG	GLN	A	90	41.964	135.303	32.480	1.00	104.28	A	C
ATOM	208	CD	GLN	A	90	43.070	135.958	33.265	1.00	105.52	A	C
ATOM	209	OE1	GLN	A	90	44.230	135.555	33.178	1.00	107.81	A	O

ATOM	210	NE2	GLN	A	90	42.721	136.978	34.041	1.00106.37	A	N
ATOM	211	C	GLN	A	90	41.044	133.396	30.550	1.00 66.25	A	C
ATOM	212	O	GLN	A	90	42.070	132.895	30.100	1.00 66.96	A	O
ATOM	213	N	HIS	A	91	40.210	134.119	29.808	1.00120.02	A	N
ATOM	214	CA	HIS	A	91	40.532	134.373	28.414	1.00120.92	A	C
ATOM	215	CB	HIS	A	91	39.487	135.272	27.747	1.00 76.79	A	C
ATOM	216	CG	HIS	A	91	39.482	135.191	26.248	1.00 77.08	A	C
ATOM	217	CD2	HIS	A	91	39.892	136.072	25.305	1.00 77.69	A	C
ATOM	218	ND1	HIS	A	91	39.009	134.092	25.563	1.00 78.34	A	N
ATOM	219	CE1	HIS	A	91	39.127	134.300	24.264	1.00 79.73	A	C
ATOM	220	NE2	HIS	A	91	39.661	135.494	24.080	1.00 79.56	A	N
ATOM	221	C	HIS	A	91	41.867	135.093	28.518	1.00120.54	A	C
ATOM	222	O	HIS	A	91	42.158	135.707	29.544	1.00121.22	A	O
ATOM	223	N	ARG	A	92	42.686	135.023	27.479	1.00100.86	A	N
ATOM	224	CA	ARG	A	92	43.987	135.663	27.549	1.00 99.32	A	C
ATOM	225	CB	ARG	A	92	45.034	134.717	26.955	1.00160.49	A	C
ATOM	226	CG	ARG	A	92	44.962	133.333	27.608	1.00163.63	A	C
ATOM	227	CD	ARG	A	92	45.925	132.304	27.028	1.00165.89	A	C
ATOM	228	NE	ARG	A	92	47.310	132.550	27.412	1.00167.52	A	N
ATOM	229	CZ	ARG	A	92	48.125	133.388	26.781	1.00168.78	A	C
ATOM	230	NH1	ARG	A	92	47.695	134.062	25.724	1.00170.17	A	N
ATOM	231	NH2	ARG	A	92	49.369	133.556	27.209	1.00169.04	A	N
ATOM	232	C	ARG	A	92	44.030	137.047	26.912	1.00 96.83	A	C
ATOM	233	O	ARG	A	92	44.498	137.997	27.530	1.00 96.93	A	O
ATOM	234	N	PRO	A	93	43.538	137.186	25.672	1.00 96.35	A	N
ATOM	235	CD	PRO	A	93	43.110	136.142	24.732	1.00 72.67	A	C
ATOM	236	CA	PRO	A	93	43.546	138.492	25.010	1.00 95.47	A	C
ATOM	237	CB	PRO	A	93	43.466	138.125	23.540	1.00 72.12	A	C
ATOM	238	CG	PRO	A	93	42.563	136.952	23.572	1.00 72.52	A	C
ATOM	239	C	PRO	A	93	42.336	139.293	25.457	1.00 93.17	A	C
ATOM	240	O	PRO	A	93	41.361	139.418	24.716	1.00 92.94	A	O
ATOM	241	N	SER	A	94	42.413	139.824	26.673	1.00 45.22	A	N
ATOM	242	CA	SER	A	94	41.338	140.608	27.259	1.00 44.33	A	C
ATOM	243	CB	SER	A	94	39.983	140.017	26.894	1.00 57.85	A	C
ATOM	244	OG	SER	A	94	39.896	138.678	27.348	1.00 58.48	A	O
ATOM	245	C	SER	A	94	41.506	140.535	28.759	1.00 43.61	A	C
ATOM	246	O	SER	A	94	41.492	141.549	29.448	1.00 43.83	A	O
ATOM	247	N	GLY	A	95	41.676	139.319	29.260	1.00 87.93	A	N
ATOM	248	CA	GLY	A	95	41.839	139.130	30.687	1.00 87.12	A	C
ATOM	249	C	GLY	A	95	40.495	138.814	31.304	1.00 87.41	A	C
ATOM	250	O	GLY	A	95	40.367	138.627	32.516	1.00 88.30	A	O
ATOM	251	N	LEU	A	96	39.479	138.764	30.454	1.00 66.37	A	N
ATOM	252	CA	LEU	A	96	38.144	138.459	30.921	1.00 64.54	A	C

ATOM	253	CB	LEU	A	96	37.145	138.456	29.758	1.00	56.05	A	C
ATOM	254	CG	LEU	A	96	36.744	139.737	29.024	1.00	54.71	A	C
ATOM	255	CD1	LEU	A	96	35.836	139.377	27.834	1.00	55.16	A	C
ATOM	256	CD2	LEU	A	96	36.040	140.678	29.991	1.00	54.17	A	C
ATOM	257	C	LEU	A	96	38.137	137.081	31.562	1.00	63.31	A	C
ATOM	258	O	LEU	A	96	38.462	136.085	30.916	1.00	62.79	A	O
ATOM	259	N	ILE	A	97	37.789	137.017	32.840	1.00	73.86	A	N
ATOM	260	CA	ILE	A	97	37.692	135.722	33.483	1.00	74.62	A	C
ATOM	261	CB	ILE	A	97	37.383	135.846	34.984	1.00	68.67	A	C
ATOM	262	CG2	ILE	A	97	37.047	134.480	35.557	1.00	68.07	A	C
ATOM	263	CG1	ILE	A	97	38.595	136.416	35.725	1.00	70.68	A	C
ATOM	264	CD1	ILE	A	97	39.741	135.439	35.863	1.00	71.88	A	C
ATOM	265	C	ILE	A	97	36.491	135.120	32.769	1.00	74.24	A	C
ATOM	266	O	ILE	A	97	35.781	135.816	32.051	1.00	74.16	A	O
ATOM	267	N	MET	A	98	36.258	133.834	32.946	1.00	39.66	A	N
ATOM	268	CA	MET	A	98	35.130	133.212	32.287	1.00	40.33	A	C
ATOM	269	CB	MET	A	98	35.522	132.806	30.860	1.00	43.61	A	C
ATOM	270	CG	MET	A	98	34.732	133.523	29.776	1.00	45.60	A	C
ATOM	271	SD	MET	A	98	35.730	134.459	28.595	1.00	44.38	A	S
ATOM	272	CE	MET	A	98	35.283	133.641	27.060	1.00	45.27	A	C
ATOM	273	C	MET	A	98	34.671	131.995	33.061	1.00	40.37	A	C
ATOM	274	O	MET	A	98	35.121	131.740	34.179	1.00	40.10	A	O
ATOM	275	N	ALA	A	99	33.743	131.265	32.462	1.00	32.92	A	N
ATOM	276	CA	ALA	A	99	33.228	130.039	33.037	1.00	31.07	A	C
ATOM	277	CB	ALA	A	99	31.842	130.254	33.614	1.00	4.67	A	C
ATOM	278	C	ALA	A	99	33.182	129.118	31.829	1.00	29.43	A	C
ATOM	279	O	ALA	A	99	32.546	129.425	30.812	1.00	28.56	A	O
ATOM	280	N	ARG	A	100	33.908	128.014	31.916	1.00	78.51	A	N
ATOM	281	CA	ARG	A	100	33.950	127.072	30.817	1.00	78.40	A	C
ATOM	282	CB	ARG	A	100	35.391	126.855	30.352	1.00	68.52	A	C
ATOM	283	CG	ARG	A	100	35.524	125.953	29.140	1.00	67.18	A	C
ATOM	284	CD	ARG	A	100	36.883	125.290	29.148	1.00	67.72	A	C
ATOM	285	NE	ARG	A	100	37.189	124.584	27.907	1.00	68.34	A	N
ATOM	286	CZ	ARG	A	100	37.397	125.182	26.739	1.00	68.25	A	C
ATOM	287	NH1	ARG	A	100	37.328	126.501	26.647	1.00	67.33	A	N
ATOM	288	NH2	ARG	A	100	37.692	124.466	25.667	1.00	67.11	A	N
ATOM	289	C	ARG	A	100	33.350	125.759	31.265	1.00	78.98	A	C
ATOM	290	O	ARG	A	100	33.948	125.017	32.045	1.00	75.97	A	O
ATOM	291	N	LYS	A	101	32.143	125.495	30.788	1.00	42.29	A	N
ATOM	292	CA	LYS	A	101	31.457	124.261	31.107	1.00	42.92	A	C
ATOM	293	CB	LYS	A	101	29.952	124.508	31.311	1.00	40.90	A	C
ATOM	294	CG	LYS	A	101	29.083	123.244	31.280	1.00	41.06	A	C
ATOM	295	CD	LYS	A	101	27.652	123.523	31.702	1.00	40.43	A	C

ATOM	296	CE	LYS A 101	27.649	124.024	33.124	1.00	40.31	A	C
ATOM	297	NZ	LYS A 101	28.573	123.208	33.972	1.00	40.19	A	N
ATOM	298	C	LYS A 101	31.705	123.326	29.934	1.00	44.28	A	C
ATOM	299	O	LYS A 101	31.234	123.554	28.815	1.00	42.69	A	O
ATOM	300	N	LEU A 102	32.469	122.277	30.200	1.00	57.28	A	N
ATOM	301	CA	LEU A 102	32.805	121.306	29.179	1.00	60.21	A	C
ATOM	302	CB	LEU A 102	34.212	120.755	29.435	1.00	94.89	A	C
ATOM	303	CG	LEU A 102	35.319	121.794	29.668	1.00	96.25	A	C
ATOM	304	CD1	LEU A 102	35.194	122.366	31.074	1.00	94.82	A	C
ATOM	305	CD2	LEU A 102	36.687	121.149	29.484	1.00	96.99	A	C
ATOM	306	C	LEU A 102	31.784	120.176	29.144	1.00	62.02	A	C
ATOM	307	O	LEU A 102	31.554	119.481	30.132	1.00	62.82	A	O
ATOM	308	N	ILE A 103	31.169	120.005	27.987	1.00	28.51	A	N
ATOM	309	CA	ILE A 103	30.172	118.975	27.813	1.00	29.87	A	C
ATOM	310	CB	ILE A 103	28.867	119.558	27.263	1.00	22.71	A	C
ATOM	311	CG2	ILE A 103	27.789	118.499	27.254	1.00	20.90	A	C
ATOM	312	CG1	ILE A 103	28.432	120.752	28.105	1.00	24.28	A	C
ATOM	313	CD1	ILE A 103	27.176	121.390	27.607	1.00	23.84	A	C
ATOM	314	C	ILE A 103	30.634	117.895	26.843	1.00	32.46	A	C
ATOM	315	O	ILE A 103	30.425	118.012	25.625	1.00	33.69	A	O
ATOM	316	N	HIS A 104	31.259	116.848	27.386	1.00	51.64	A	N
ATOM	317	CA	HIS A 104	31.721	115.709	26.587	1.00	53.00	A	C
ATOM	318	CB	HIS A 104	32.494	114.710	27.460	1.00	192.39	A	C
ATOM	319	CG	HIS A 104	33.983	114.848	27.379	1.00	192.22	A	C
ATOM	320	CD2	HIS A 104	34.924	114.036	26.841	1.00	193.15	A	C
ATOM	321	ND1	HIS A 104	34.664	115.927	27.903	1.00	191.98	A	N
ATOM	322	CE1	HIS A 104	35.959	115.771	27.693	1.00	192.89	A	C
ATOM	323	NE2	HIS A 104	36.144	114.632	27.050	1.00	193.47	A	N
ATOM	324	C	HIS A 104	30.516	114.998	25.960	1.00	54.27	A	C
ATOM	325	O	HIS A 104	29.974	114.055	26.520	1.00	54.09	A	O
ATOM	326	N	LEU A 105	30.089	115.459	24.796	1.00	58.86	A	N
ATOM	327	CA	LEU A 105	28.956	114.840	24.141	1.00	59.27	A	C
ATOM	328	CB	LEU A 105	28.068	115.908	23.513	1.00	151.52	A	C
ATOM	329	CG	LEU A 105	27.405	116.795	24.562	1.00	153.49	A	C
ATOM	330	CD1	LEU A 105	26.619	117.910	23.898	1.00	153.90	A	C
ATOM	331	CD2	LEU A 105	26.507	115.931	25.428	1.00	153.15	A	C
ATOM	332	C	LEU A 105	29.410	113.854	23.083	1.00	60.93	A	C
ATOM	333	O	LEU A 105	29.770	114.237	21.963	1.00	58.49	A	O
ATOM	334	N	GLU A 106	29.416	112.577	23.449	1.00	97.60	A	N
ATOM	335	CA	GLU A 106	29.804	111.550	22.506	1.00	99.97	A	C
ATOM	336	CB	GLU A 106	29.838	110.171	23.170	1.00	203.67	A	C
ATOM	337	CG	GLU A 106	30.439	109.085	22.284	1.00	203.67	A	C
ATOM	338	CD	GLU A 106	31.924	109.290	22.016	1.00	203.67	A	C

ATOM	339	OE1	GLU	A	106	32.316	110.401	21.596	1.00203.67	A	O
ATOM	340	OE2	GLU	A	106	32.700	108.333	22.219	1.00203.67	A	O
ATOM	341	C	GLU	A	106	28.720	111.607	21.440	1.00100.72	A	C
ATOM	342	O	GLU	A	106	27.552	111.297	21.701	1.00100.41	A	O
ATOM	343	N	ILE	A	107	29.110	112.037	20.250	1.00 88.26	A	N
ATOM	344	CA	ILE	A	107	28.183	112.160	19.148	1.00 89.67	A	C
ATOM	345	CB	ILE	A	107	27.194	113.323	19.402	1.00157.96	A	C
ATOM	346	CG2	ILE	A	107	27.948	114.653	19.432	1.00156.74	A	C
ATOM	347	CG1	ILE	A	107	26.103	113.332	18.330	1.00160.27	A	C
ATOM	348	CD1	ILE	A	107	25.246	112.069	18.300	1.00161.75	A	C
ATOM	349	C	ILE	A	107	28.944	112.393	17.835	1.00 89.73	A	C
ATOM	350	O	ILE	A	107	30.017	113.022	17.833	1.00 89.13	A	O
ATOM	351	N	LYS	A	108	28.401	111.892	16.748	1.00 87.28	A	N
ATOM	352	CA	LYS	A	108	29.036	112.039	15.441	1.00 88.15	A	C
ATOM	353	CB	LYS	A	108	28.491	110.994	14.465	1.00138.97	A	C
ATOM	354	CG	LYS	A	108	28.796	109.555	14.837	1.00140.15	A	C
ATOM	355	CD	LYS	A	108	28.336	108.611	13.737	1.00141.41	A	C
ATOM	356	CE	LYS	A	108	28.535	107.152	14.119	1.00142.51	A	C
ATOM	357	NZ	LYS	A	108	27.697	106.728	15.279	1.00143.21	A	N
ATOM	358	C	LYS	A	108	28.867	113.421	14.831	1.00 86.89	A	C
ATOM	359	O	LYS	A	108	27.774	113.802	14.429	1.00 87.82	A	O
ATOM	360	N	PRO	A	109	29.974	114.174	14.736	1.00 57.42	A	N
ATOM	361	CD	PRO	A	109	31.279	113.565	15.066	1.00119.11	A	C
ATOM	362	CA	PRO	A	109	30.168	115.529	14.212	1.00 57.17	A	C
ATOM	363	CB	PRO	A	109	31.600	115.471	13.711	1.00118.30	A	C
ATOM	364	CG	PRO	A	109	32.243	114.721	14.822	1.00118.00	A	C
ATOM	365	C	PRO	A	109	29.176	115.959	13.128	1.00 55.61	A	C
ATOM	366	O	PRO	A	109	28.751	117.122	13.065	1.00 56.03	A	O
ATOM	367	N	ALA	A	110	28.818	114.990	12.284	1.00110.62	A	N
ATOM	368	CA	ALA	A	110	27.884	115.189	11.188	1.00110.97	A	C
ATOM	369	CB	ALA	A	110	27.101	113.879	10.928	1.00 62.46	A	C
ATOM	370	C	ALA	A	110	26.899	116.351	11.384	1.00109.04	A	C
ATOM	371	O	ALA	A	110	26.991	117.365	10.691	1.00107.81	A	O
ATOM	372	N	ILE	A	111	25.966	116.205	12.311	1.00190.06	A	N
ATOM	373	CA	ILE	A	111	24.968	117.249	12.530	1.00189.32	A	C
ATOM	374	CB	ILE	A	111	23.529	116.643	12.684	1.00 78.88	A	C
ATOM	375	CG2	ILE	A	111	23.236	115.679	11.518	1.00 79.41	A	C
ATOM	376	CG1	ILE	A	111	23.387	115.905	14.030	1.00 80.16	A	C
ATOM	377	CD1	ILE	A	111	22.932	116.775	15.178	1.00 81.58	A	C
ATOM	378	C	ILE	A	111	25.273	118.104	13.753	1.00187.30	A	C
ATOM	379	O	ILE	A	111	24.652	119.146	13.939	1.00185.38	A	O
ATOM	380	N	ARG	A	112	26.229	117.661	14.565	1.00 87.18	A	N
ATOM	381	CA	ARG	A	112	26.618	118.359	15.795	1.00 88.54	A	C

ATOM	382	CB	ARG	A	112	28.004	117.879	16.269	1.00 82.15	A	C
ATOM	383	CG	ARG	A	112	29.079	118.984	16.318	1.00 82.66	A	C
ATOM	384	CD	ARG	A	112	30.475	118.411	16.216	1.00 83.36	A	C
ATOM	385	NE	ARG	A	112	31.169	119.013	15.082	1.00 85.67	A	N
ATOM	386	CZ	ARG	A	112	32.343	118.605	14.622	1.00 86.98	A	C
ATOM	387	NH1	ARG	A	112	32.900	119.218	13.584	1.00 87.20	A	N
ATOM	388	NH2	ARG	A	112	32.957	117.581	15.203	1.00 87.68	A	N
ATOM	389	C	ARG	A	112	26.655	119.865	15.667	1.00 88.24	A	C
ATOM	390	O	ARG	A	112	26.284	120.577	16.603	1.00 88.17	A	O
ATOM	391	N	ASN	A	113	27.111	120.352	14.524	1.00136.92	A	N
ATOM	392	CA	ASN	A	113	27.206	121.782	14.329	1.00138.08	A	C
ATOM	393	CB	ASN	A	113	27.685	122.156	12.910	1.00171.85	A	C
ATOM	394	CG	ASN	A	113	28.332	120.983	12.163	1.00171.77	A	C
ATOM	395	OD1	ASN	A	113	29.013	120.130	12.738	1.00171.91	A	O
ATOM	396	ND2	ASN	A	113	28.130	120.966	10.846	1.00171.41	A	N
ATOM	397	C	ASN	A	113	25.836	122.377	14.611	1.00138.72	A	C
ATOM	398	O	ASN	A	113	25.722	123.511	15.055	1.00138.47	A	O
ATOM	399	N	GLN	A	114	24.799	121.583	14.359	1.00133.26	A	N
ATOM	400	CA	GLN	A	114	23.419	121.973	14.614	1.00133.48	A	C
ATOM	401	CB	GLN	A	114	22.488	120.800	14.324	1.00 75.04	A	C
ATOM	402	CG	GLN	A	114	21.037	121.095	14.548	1.00 78.76	A	C
ATOM	403	CD	GLN	A	114	20.186	119.875	14.426	1.00 82.05	A	C
ATOM	404	OE1	GLN	A	114	19.004	119.899	14.740	1.00 83.03	A	O
ATOM	405	NE2	GLN	A	114	20.780	118.787	13.961	1.00 83.78	A	N
ATOM	406	C	GLN	A	114	23.282	122.369	16.097	1.00131.58	A	C
ATOM	407	O	GLN	A	114	22.265	122.946	16.490	1.00129.92	A	O
ATOM	408	N	ILE	A	115	24.281	122.073	16.893	1.00 65.62	A	N
ATOM	409	CA	ILE	A	115	24.253	122.377	18.327	1.00 62.15	A	C
ATOM	410	CB	ILE	A	115	25.004	121.285	19.137	1.00 45.96	A	C
ATOM	411	CG2	ILE	A	115	25.573	121.866	20.444	1.00 44.90	A	C
ATOM	412	CG1	ILE	A	115	24.089	120.062	19.289	1.00 46.07	A	C
ATOM	413	CD1	ILE	A	115	24.662	119.006	20.182	1.00 47.57	A	C
ATOM	414	C	ILE	A	115	24.872	123.719	18.573	1.00 62.14	A	C
ATOM	415	O	ILE	A	115	24.350	124.516	19.345	1.00 61.44	A	O
ATOM	416	N	ILE	A	116	26.006	123.981	17.950	1.00 52.01	A	N
ATOM	417	CA	ILE	A	116	26.619	125.285	18.122	1.00 51.07	A	C
ATOM	418	CB	ILE	A	116	28.072	125.357	17.590	1.00 55.07	A	C
ATOM	419	CG2	ILE	A	116	28.621	126.765	17.723	1.00 55.00	A	C
ATOM	420	CG1	ILE	A	116	28.974	124.453	18.419	1.00 56.57	A	C
ATOM	421	CD1	ILE	A	116	28.639	122.993	18.317	1.00 58.61	A	C
ATOM	422	C	ILE	A	116	25.722	126.248	17.347	1.00 51.72	A	C
ATOM	423	O	ILE	A	116	25.526	127.395	17.754	1.00 51.77	A	O
ATOM	424	N	ARG	A	117	25.160	125.753	16.245	1.00 70.65	A	N

ATOM	425	CA	ARG	A	117	24.255	126.538	15.419	1.00	69.60	A	C
ATOM	426	CB	ARG	A	117	23.728	125.715	14.247	1.00	65.91	A	C
ATOM	427	CG	ARG	A	117	22.621	126.411	13.472	1.00	68.37	A	C
ATOM	428	CD	ARG	A	117	21.780	125.433	12.654	1.00	72.75	A	C
ATOM	429	NE	ARG	A	117	20.548	126.054	12.156	1.00	76.75	A	N
ATOM	430	CZ	ARG	A	117	20.453	126.791	11.048	1.00	78.33	A	C
ATOM	431	NH1	ARG	A	117	21.523	127.010	10.290	1.00	78.17	A	N
ATOM	432	NH2	ARG	A	117	19.282	127.315	10.699	1.00	79.41	A	N
ATOM	433	C	ARG	A	117	23.093	126.926	16.316	1.00	68.33	A	C
ATOM	434	O	ARG	A	117	22.778	128.106	16.477	1.00	68.99	A	O
ATOM	435	N	GLU	A	118	22.456	125.928	16.916	1.00	88.35	A	N
ATOM	436	CA	GLU	A	118	21.338	126.217	17.799	1.00	86.50	A	C
ATOM	437	CB	GLU	A	118	20.692	124.913	18.295	1.00	89.15	A	C
ATOM	438	CG	GLU	A	118	19.863	124.168	17.240	1.00	89.91	A	C
ATOM	439	CD	GLU	A	118	19.118	122.962	17.807	1.00	90.63	A	C
ATOM	440	OE1	GLU	A	118	18.302	123.145	18.729	1.00	89.94	A	O
ATOM	441	OE2	GLU	A	118	19.340	121.828	17.334	1.00	90.54	A	O
ATOM	442	C	GLU	A	118	21.817	127.074	18.978	1.00	84.07	A	C
ATOM	443	O	GLU	A	118	21.202	128.088	19.321	1.00	83.43	A	O
ATOM	444	N	LEU	A	119	22.936	126.672	19.574	1.00	44.43	A	N
ATOM	445	CA	LEU	A	119	23.509	127.378	20.708	1.00	40.61	A	C
ATOM	446	CB	LEU	A	119	24.782	126.683	21.185	1.00	38.74	A	C
ATOM	447	CG	LEU	A	119	24.615	125.543	22.183	1.00	37.45	A	C
ATOM	448	CD1	LEU	A	119	25.971	125.024	22.589	1.00	38.08	A	C
ATOM	449	CD2	LEU	A	119	23.885	126.034	23.406	1.00	38.25	A	C
ATOM	450	C	LEU	A	119	23.836	128.829	20.437	1.00	40.66	A	C
ATOM	451	O	LEU	A	119	24.324	129.516	21.325	1.00	41.33	A	O
ATOM	452	N	GLN	A	120	23.575	129.305	19.228	1.00	62.19	A	N
ATOM	453	CA	GLN	A	120	23.889	130.690	18.905	1.00	62.47	A	C
ATOM	454	CB	GLN	A	120	24.137	130.830	17.408	1.00	44.16	A	C
ATOM	455	CG	GLN	A	120	25.471	130.269	17.008	1.00	45.80	A	C
ATOM	456	CD	GLN	A	120	26.587	130.799	17.892	1.00	46.88	A	C
ATOM	457	OE1	GLN	A	120	26.732	132.010	18.054	1.00	47.02	A	O
ATOM	458	NE2	GLN	A	120	27.380	129.897	18.467	1.00	46.18	A	N
ATOM	459	C	GLN	A	120	22.865	131.721	19.363	1.00	60.45	A	C
ATOM	460	O	GLN	A	120	23.214	132.870	19.625	1.00	59.07	A	O
ATOM	461	N	VAL	A	121	21.607	131.316	19.472	1.00	36.12	A	N
ATOM	462	CA	VAL	A	121	20.561	132.230	19.902	1.00	35.49	A	C
ATOM	463	CB	VAL	A	121	19.217	131.506	20.038	1.00	96.62	A	C
ATOM	464	CG1	VAL	A	121	19.019	130.568	18.858	1.00	98.72	A	C
ATOM	465	CG2	VAL	A	121	19.162	130.756	21.363	1.00	98.97	A	C
ATOM	466	C	VAL	A	121	20.897	132.849	21.252	1.00	32.85	A	C
ATOM	467	O	VAL	A	121	20.190	133.728	21.735	1.00	30.62	A	O

ATOM	468	N	LEU	A	122	21.978	132.380	21.860	1.00	40.57	A	N
ATOM	469	CA	LEU	A	122	22.397	132.882	23.157	1.00	38.34	A	C
ATOM	470	CB	LEU	A	122	23.408	131.926	23.780	1.00	52.23	A	C
ATOM	471	CG	LEU	A	122	22.785	130.695	24.429	1.00	52.21	A	C
ATOM	472	CD1	LEU	A	122	23.852	129.808	25.060	1.00	51.08	A	C
ATOM	473	CD2	LEU	A	122	21.806	131.177	25.487	1.00	51.40	A	C
ATOM	474	C	LEU	A	122	22.974	134.281	23.080	1.00	35.40	A	C
ATOM	475	O	LEU	A	122	23.087	134.976	24.085	1.00	34.19	A	O
ATOM	476	N	HIS	A	123	23.336	134.702	21.880	1.00	34.03	A	N
ATOM	477	CA	HIS	A	123	23.889	136.034	21.703	1.00	34.71	A	C
ATOM	478	CB	HIS	A	123	24.701	136.086	20.415	1.00	29.62	A	C
ATOM	479	CG	HIS	A	123	26.073	135.508	20.562	1.00	27.02	A	C
ATOM	480	CD2	HIS	A	123	26.939	135.526	21.603	1.00	26.42	A	C
ATOM	481	ND1	HIS	A	123	26.712	134.832	19.546	1.00	27.19	A	N
ATOM	482	CE1	HIS	A	123	27.912	134.458	19.954	1.00	27.44	A	C
ATOM	483	NE2	HIS	A	123	28.075	134.867	21.199	1.00	26.90	A	N
ATOM	484	C	HIS	A	123	22.759	137.039	21.696	1.00	36.88	A	C
ATOM	485	O	HIS	A	123	22.958	138.213	21.971	1.00	36.10	A	O
ATOM	486	N	GLU	A	124	21.562	136.554	21.406	1.00	18.26	A	N
ATOM	487	CA	GLU	A	124	20.396	137.401	21.390	1.00	19.99	A	C
ATOM	488	CB	GLU	A	124	19.345	136.842	20.438	1.00	99.84	A	C
ATOM	489	CG	GLU	A	124	19.845	136.683	19.030	1.00	105.65	A	C
ATOM	490	CD	GLU	A	124	20.262	138.000	18.419	1.00	109.81	A	C
ATOM	491	OE1	GLU	A	124	20.922	137.969	17.359	1.00	112.87	A	O
ATOM	492	OE2	GLU	A	124	19.926	139.063	18.989	1.00	111.16	A	O
ATOM	493	C	GLU	A	124	19.823	137.470	22.796	1.00	22.12	A	C
ATOM	494	O	GLU	A	124	19.114	138.424	23.125	1.00	24.01	A	O
ATOM	495	N	CYS	A	125	20.141	136.463	23.619	1.00	46.56	A	N
ATOM	496	CA	CYS	A	125	19.658	136.369	25.005	1.00	46.88	A	C
ATOM	497	CB	CYS	A	125	19.895	134.986	25.578	1.00	26.51	A	C
ATOM	498	SG	CYS	A	125	18.802	133.729	25.056	1.00	29.07	A	S
ATOM	499	C	CYS	A	125	20.331	137.318	25.955	1.00	44.97	A	C
ATOM	500	O	CYS	A	125	21.395	137.004	26.483	1.00	46.02	A	O
ATOM	501	N	ASN	A	126	19.716	138.460	26.213	1.00	59.62	A	N
ATOM	502	CA	ASN	A	126	20.323	139.398	27.132	1.00	61.39	A	C
ATOM	503	CB	ASN	A	126	21.228	140.367	26.360	1.00	86.54	A	C
ATOM	504	CG	ASN	A	126	22.571	139.731	25.977	1.00	88.51	A	C
ATOM	505	OD1	ASN	A	126	23.347	139.325	26.846	1.00	87.95	A	O
ATOM	506	ND2	ASN	A	126	22.842	139.640	24.679	1.00	88.39	A	N
ATOM	507	C	ASN	A	126	19.314	140.141	28.004	1.00	60.55	A	C
ATOM	508	O	ASN	A	126	18.611	141.038	27.548	1.00	61.27	A	O
ATOM	509	N	SER	A	127	19.250	139.721	29.267	1.00	20.51	A	N
ATOM	510	CA	SER	A	127	18.375	140.288	30.285	1.00	18.01	A	C

ATOM	511	CB	SER	A	127	17.167	139.376	30.494	1.00 32.92	A	C
ATOM	512	OG	SER	A	127	16.406	139.752	31.629	1.00 33.29	A	O
ATOM	513	C	SER	A	127	19.216	140.322	31.548	1.00 18.24	A	C
ATOM	514	O	SER	A	127	20.160	139.566	31.674	1.00 21.10	A	O
ATOM	515	N	PRO	A	128	18.901	141.201	32.500	1.00 39.21	A	N
ATOM	516	CD	PRO	A	128	17.843	142.225	32.544	1.00 41.28	A	C
ATOM	517	CA	PRO	A	128	19.713	141.230	33.724	1.00 39.51	A	C
ATOM	518	CB	PRO	A	128	19.313	142.549	34.364	1.00 41.81	A	C
ATOM	519	CG	PRO	A	128	17.845	142.628	34.011	1.00 40.66	A	C
ATOM	520	C	PRO	A	128	19.378	140.046	34.622	1.00 37.87	A	C
ATOM	521	O	PRO	A	128	19.581	140.082	35.830	1.00 38.86	A	O
ATOM	522	N	TYR	A	129	18.859	138.995	34.018	1.00 24.94	A	N
ATOM	523	CA	TYR	A	129	18.469	137.837	34.771	1.00 23.80	A	C
ATOM	524	CB	TYR	A	129	16.947	137.832	34.892	1.00 31.68	A	C
ATOM	525	CG	TYR	A	129	16.420	139.073	35.570	1.00 31.86	A	C
ATOM	526	CD1	TYR	A	129	17.001	139.532	36.736	1.00 33.86	A	C
ATOM	527	CE1	TYR	A	129	16.560	140.693	37.348	1.00 34.92	A	C
ATOM	528	CD2	TYR	A	129	15.371	139.804	35.033	1.00 31.61	A	C
ATOM	529	CE2	TYR	A	129	14.920	140.972	35.646	1.00 32.41	A	C
ATOM	530	CZ	TYR	A	129	15.524	141.409	36.802	1.00 33.41	A	C
ATOM	531	OH	TYR	A	129	15.122	142.566	37.424	1.00 33.43	A	O
ATOM	532	C	TYR	A	129	18.981	136.540	34.153	1.00 23.99	A	C
ATOM	533	O	TYR	A	129	18.774	135.462	34.705	1.00 25.69	A	O
ATOM	534	N	ILE	A	130	19.632	136.641	32.998	1.00 30.30	A	N
ATOM	535	CA	ILE	A	130	20.196	135.474	32.336	1.00 30.47	A	C
ATOM	536	CB	ILE	A	130	19.514	135.158	31.003	1.00 41.94	A	C
ATOM	537	CG2	ILE	A	130	20.378	134.200	30.219	1.00 43.21	A	C
ATOM	538	CG1	ILE	A	130	18.162	134.490	31.236	1.00 41.91	A	C
ATOM	539	CD1	ILE	A	130	17.165	135.350	31.927	1.00 46.10	A	C
ATOM	540	C	ILE	A	130	21.676	135.697	32.073	1.00 28.68	A	C
ATOM	541	O	ILE	A	130	22.074	136.660	31.424	1.00 27.48	A	O
ATOM	542	N	VAL	A	131	22.483	134.781	32.583	1.00 24.17	A	N
ATOM	543	CA	VAL	A	131	23.931	134.816	32.465	1.00 24.06	A	C
ATOM	544	CB	VAL	A	131	24.491	133.493	32.941	1.00 12.82	A	C
ATOM	545	CG1	VAL	A	131	25.902	133.312	32.467	1.00 12.22	A	C
ATOM	546	CG2	VAL	A	131	24.425	133.467	34.447	1.00 11.74	A	C
ATOM	547	C	VAL	A	131	24.521	135.151	31.106	1.00 26.00	A	C
ATOM	548	O	VAL	A	131	23.961	134.827	30.069	1.00 24.82	A	O
ATOM	549	N	GLY	A	132	25.672	135.806	31.124	1.00 53.27	A	N
ATOM	550	CA	GLY	A	132	26.319	136.176	29.885	1.00 58.26	A	C
ATOM	551	C	GLY	A	132	26.707	134.986	29.034	1.00 62.37	A	C
ATOM	552	O	GLY	A	132	26.847	133.865	29.528	1.00 64.19	A	O
ATOM	553	N	PHE	A	133	26.878	135.238	27.742	1.00 39.62	A	N

ATOM	554	CA	PHE	A	133	27.262	134.195	26.810	1.00	41.34	A	C
ATOM	555	CB	PHE	A	133	26.070	133.758	25.970	1.00	45.32	A	C
ATOM	556	CG	PHE	A	133	26.410	132.718	24.936	1.00	47.44	A	C
ATOM	557	CD1	PHE	A	133	26.867	131.466	25.315	1.00	48.46	A	C
ATOM	558	CD2	PHE	A	133	26.275	132.990	23.588	1.00	49.55	A	C
ATOM	559	CE1	PHE	A	133	27.180	130.507	24.371	1.00	49.76	A	C
ATOM	560	CE2	PHE	A	133	26.587	132.034	22.642	1.00	49.98	A	C
ATOM	561	CZ	PHE	A	133	27.040	130.792	23.037	1.00	50.60	A	C
ATOM	562	C	PHE	A	133	28.373	134.644	25.880	1.00	41.29	A	C
ATOM	563	O	PHE	A	133	28.120	135.289	24.862	1.00	42.43	A	O
ATOM	564	N	TYR	A	134	29.608	134.294	26.223	1.00	37.59	A	N
ATOM	565	CA	TYR	A	134	30.737	134.661	25.391	1.00	38.30	A	C
ATOM	566	CB	TYR	A	134	32.032	134.541	26.163	1.00	37.67	A	C
ATOM	567	CG	TYR	A	134	32.161	135.480	27.316	1.00	38.57	A	C
ATOM	568	CD1	TYR	A	134	31.798	135.090	28.600	1.00	38.56	A	C
ATOM	569	CE1	TYR	A	134	31.991	135.937	29.684	1.00	37.63	A	C
ATOM	570	CD2	TYR	A	134	32.710	136.745	27.139	1.00	38.75	A	C
ATOM	571	CE2	TYR	A	134	32.905	137.600	28.213	1.00	38.46	A	C
ATOM	572	CZ	TYR	A	134	32.549	137.188	29.480	1.00	38.08	A	C
ATOM	573	OH	TYR	A	134	32.782	138.017	30.548	1.00	39.20	A	O
ATOM	574	C	TYR	A	134	30.855	133.809	24.134	1.00	38.98	A	C
ATOM	575	O	TYR	A	134	31.422	134.250	23.144	1.00	40.23	A	O
ATOM	576	N	GLY	A	135	30.340	132.586	24.163	1.00	66.72	A	N
ATOM	577	CA	GLY	A	135	30.453	131.755	22.978	1.00	68.14	A	C
ATOM	578	C	GLY	A	135	30.496	130.269	23.229	1.00	68.29	A	C
ATOM	579	O	GLY	A	135	30.655	129.801	24.362	1.00	67.51	A	O
ATOM	580	N	ALA	A	136	30.357	129.534	22.129	1.00	114.41	A	N
ATOM	581	CA	ALA	A	136	30.346	128.078	22.140	1.00	116.31	A	C
ATOM	582	CB	ALA	A	136	28.907	127.572	22.100	1.00	140.32	A	C
ATOM	583	C	ALA	A	136	31.081	127.578	20.906	1.00	116.09	A	C
ATOM	584	O	ALA	A	136	31.163	128.288	19.906	1.00	116.90	A	O
ATOM	585	N	PHE	A	137	31.634	126.374	20.968	1.00	100.40	A	N
ATOM	586	CA	PHE	A	137	32.291	125.842	19.795	1.00	101.65	A	C
ATOM	587	CB	PHE	A	137	33.701	126.384	19.658	1.00	51.69	A	C
ATOM	588	CG	PHE	A	137	34.396	126.603	20.949	1.00	50.20	A	C
ATOM	589	CD1	PHE	A	137	34.255	127.797	21.649	1.00	48.83	A	C
ATOM	590	CD2	PHE	A	137	35.200	125.615	21.470	1.00	49.63	A	C
ATOM	591	CE1	PHE	A	137	34.930	127.998	22.856	1.00	49.79	A	C
ATOM	592	CE2	PHE	A	137	35.875	125.803	22.673	1.00	49.70	A	C
ATOM	593	CZ	PHE	A	137	35.744	126.997	23.367	1.00	49.20	A	C
ATOM	594	C	PHE	A	137	32.308	124.326	19.780	1.00	104.51	A	C
ATOM	595	O	PHE	A	137	31.267	123.668	19.927	1.00	104.42	A	O
ATOM	596	N	TYR	A	138	33.485	123.763	19.598	1.00	197.50	A	N

ATOM	597	CA	TYR	A	138	33.589	122.326	19.528	1.00200.36	A	C
ATOM	598	CB	TYR	A	138	33.438	121.871	18.064	1.00203.13	A	C
ATOM	599	CG	TYR	A	138	33.970	122.838	17.007	1.00203.13	A	C
ATOM	600	CD1	TYR	A	138	34.792	122.383	15.985	1.00203.13	A	C
ATOM	601	CE1	TYR	A	138	35.299	123.247	15.029	1.00203.13	A	C
ATOM	602	CD2	TYR	A	138	33.663	124.199	17.036	1.00203.13	A	C
ATOM	603	CE2	TYR	A	138	34.167	125.073	16.086	1.00203.13	A	C
ATOM	604	CZ	TYR	A	138	34.988	124.591	15.086	1.00203.13	A	C
ATOM	605	OH	TYR	A	138	35.519	125.454	14.153	1.00203.13	A	O
ATOM	606	C	TYR	A	138	34.897	121.855	20.117	1.00202.81	A	C
ATOM	607	O	TYR	A	138	35.078	121.900	21.334	1.00202.56	A	O
ATOM	608	N	SER	A	139	35.795	121.423	19.242	1.00176.35	A	N
ATOM	609	CA	SER	A	139	37.115	120.916	19.609	1.00178.55	A	C
ATOM	610	CB	SER	A	139	37.309	120.896	21.128	1.00167.15	A	C
ATOM	611	OG	SER	A	139	38.603	120.450	21.471	1.00167.47	A	O
ATOM	612	C	SER	A	139	37.227	119.500	19.069	1.00178.84	A	C
ATOM	613	O	SER	A	139	36.834	119.241	17.928	1.00178.83	A	O
ATOM	614	N	ASP	A	140	37.750	118.584	19.878	1.00178.63	A	N
ATOM	615	CA	ASP	A	140	37.901	117.198	19.453	1.00179.43	A	C
ATOM	616	CB	ASP	A	140	39.289	116.955	18.865	1.00173.23	A	C
ATOM	617	CG	ASP	A	140	39.400	115.627	18.134	1.00175.19	A	C
ATOM	618	OD1	ASP	A	140	38.366	114.926	18.020	1.00175.60	A	O
ATOM	619	OD2	ASP	A	140	40.502	115.282	17.670	1.00176.80	A	O
ATOM	620	C	ASP	A	140	37.680	116.263	20.633	1.00178.50	A	C
ATOM	621	O	ASP	A	140	38.484	115.365	20.898	1.00178.52	A	O
ATOM	622	N	GLY	A	141	36.582	116.486	21.342	1.00149.44	A	N
ATOM	623	CA	GLY	A	141	36.276	115.658	22.484	1.00147.42	A	C
ATOM	624	C	GLY	A	141	35.615	116.402	23.628	1.00145.22	A	C
ATOM	625	O	GLY	A	141	35.848	116.074	24.794	1.00146.30	A	O
ATOM	626	N	GLU	A	142	34.805	117.395	23.307	1.00 75.48	A	N
ATOM	627	CA	GLU	A	142	34.104	118.150	24.342	1.00 71.63	A	C
ATOM	628	CB	GLU	A	142	35.054	118.459	25.502	1.00203.67	A	C
ATOM	629	CG	GLU	A	142	34.610	119.559	26.441	1.00203.67	A	C
ATOM	630	CD	GLU	A	142	35.317	120.853	26.125	1.00203.67	A	C
ATOM	631	OE1	GLU	A	142	36.478	120.772	25.675	1.00203.67	A	O
ATOM	632	OE2	GLU	A	142	34.736	121.938	26.325	1.00203.67	A	O
ATOM	633	C	GLU	A	142	33.470	119.432	23.842	1.00 68.49	A	C
ATOM	634	O	GLU	A	142	34.067	120.164	23.060	1.00 68.37	A	O
ATOM	635	N	ILE	A	143	32.242	119.681	24.278	1.00 55.15	A	N
ATOM	636	CA	ILE	A	143	31.534	120.902	23.913	1.00 50.81	A	C
ATOM	637	CB	ILE	A	143	30.044	120.715	23.862	1.00 24.95	A	C
ATOM	638	CG2	ILE	A	143	29.379	121.992	24.346	1.00 22.99	A	C
ATOM	639	CG1	ILE	A	143	29.599	120.445	22.425	1.00 26.47	A	C

ATOM	640	CD1	ILE	A	143	29.381	121.723	21.611	1.00	29.74	A	C
ATOM	641	C	ILE	A	143	31.794	121.935	24.986	1.00	48.71	A	C
ATOM	642	O	ILE	A	143	31.694	121.640	26.185	1.00	46.48	A	O
ATOM	643	N	SER	A	144	32.111	123.149	24.572	1.00	48.84	A	N
ATOM	644	CA	SER	A	144	32.400	124.187	25.550	1.00	48.41	A	C
ATOM	645	CB	SER	A	144	33.905	124.498	25.577	1.00	59.42	A	C
ATOM	646	OG	SER	A	144	34.619	123.794	24.574	1.00	60.91	A	O
ATOM	647	C	SER	A	144	31.603	125.469	25.372	1.00	46.45	A	C
ATOM	648	O	SER	A	144	31.641	126.088	24.306	1.00	45.81	A	O
ATOM	649	N	ILE	A	145	30.876	125.859	26.414	1.00	29.11	A	N
ATOM	650	CA	ILE	A	145	30.058	127.064	26.439	1.00	28.12	A	C
ATOM	651	CB	ILE	A	145	28.626	126.780	26.972	1.00	18.49	A	C
ATOM	652	CG2	ILE	A	145	27.898	128.078	27.281	1.00	19.03	A	C
ATOM	653	CG1	ILE	A	145	27.824	125.963	25.963	1.00	17.94	A	C
ATOM	654	CD1	ILE	A	145	26.453	125.610	26.480	1.00	17.14	A	C
ATOM	655	C	ILE	A	145	30.735	127.991	27.421	1.00	27.52	A	C
ATOM	656	O	ILE	A	145	30.626	127.790	28.620	1.00	26.12	A	O
ATOM	657	N	CYS	A	146	31.448	128.995	26.922	1.00	39.61	A	N
ATOM	658	CA	CYS	A	146	32.121	129.939	27.793	1.00	43.33	A	C
ATOM	659	CB	CYS	A	146	33.256	130.603	27.029	1.00	54.97	A	C
ATOM	660	SG	CYS	A	146	34.357	129.377	26.342	1.00	58.71	A	S
ATOM	661	C	CYS	A	146	31.068	130.953	28.198	1.00	43.61	A	C
ATOM	662	O	CYS	A	146	30.325	131.449	27.349	1.00	44.47	A	O
ATOM	663	N	MET	A	147	30.987	131.252	29.488	1.00	45.90	A	N
ATOM	664	CA	MET	A	147	29.975	132.179	29.959	1.00	46.19	A	C
ATOM	665	CB	MET	A	147	28.789	131.402	30.531	1.00	80.46	A	C
ATOM	666	CG	MET	A	147	29.168	130.514	31.693	1.00	83.32	A	C
ATOM	667	SD	MET	A	147	28.050	129.127	31.873	1.00	87.75	A	S
ATOM	668	CE	MET	A	147	27.161	129.575	33.350	1.00	86.59	A	C
ATOM	669	C	MET	A	147	30.481	133.138	31.003	1.00	44.56	A	C
ATOM	670	O	MET	A	147	31.644	133.110	31.382	1.00	44.47	A	O
ATOM	671	N	GLU	A	148	29.567	133.979	31.461	1.00	36.34	A	N
ATOM	672	CA	GLU	A	148	29.823	134.989	32.465	1.00	34.74	A	C
ATOM	673	CB	GLU	A	148	28.655	135.977	32.428	1.00	51.33	A	C
ATOM	674	CG	GLU	A	148	28.204	136.567	33.741	1.00	52.17	A	C
ATOM	675	CD	GLU	A	148	27.141	137.619	33.517	1.00	52.82	A	C
ATOM	676	OE1	GLU	A	148	26.102	137.293	32.899	1.00	49.32	A	O
ATOM	677	OE2	GLU	A	148	27.347	138.773	33.948	1.00	53.93	A	O
ATOM	678	C	GLU	A	148	30.028	134.414	33.869	1.00	33.53	A	C
ATOM	679	O	GLU	A	148	29.091	133.924	34.502	1.00	34.73	A	O
ATOM	680	N	HIS	A	149	31.264	134.480	34.351	1.00	25.76	A	N
ATOM	681	CA	HIS	A	149	31.586	133.969	35.672	1.00	24.86	A	C
ATOM	682	CB	HIS	A	149	33.088	134.031	35.912	1.00	50.14	A	C

ATOM	683	CG	HIS	A	149	33.486	133.744	37.325	1.00	46.99	A	C
ATOM	684	CD2	HIS	A	149	33.697	132.572	37.969	1.00	44.20	A	C
ATOM	685	ND1	HIS	A	149	33.719	134.737	38.250	1.00	45.24	A	N
ATOM	686	CE1	HIS	A	149	34.061	134.190	39.402	1.00	43.11	A	C
ATOM	687	NE2	HIS	A	149	34.055	132.878	39.258	1.00	40.98	A	N
ATOM	688	C	HIS	A	149	30.881	134.746	36.763	1.00	26.23	A	C
ATOM	689	O	HIS	A	149	30.989	135.959	36.833	1.00	28.55	A	O
ATOM	690	N	MET	A	150	30.159	134.039	37.620	1.00	10.86	A	N
ATOM	691	CA	MET	A	150	29.428	134.649	38.718	1.00	11.68	A	C
ATOM	692	CB	MET	A	150	28.052	133.995	38.860	1.00	55.70	A	C
ATOM	693	CG	MET	A	150	27.201	134.046	37.604	1.00	57.05	A	C
ATOM	694	SD	MET	A	150	26.843	135.732	37.086	1.00	59.51	A	S
ATOM	695	CE	MET	A	150	25.784	136.272	38.423	1.00	56.65	A	C
ATOM	696	C	MET	A	150	30.215	134.452	39.999	1.00	11.01	A	C
ATOM	697	O	MET	A	150	30.227	133.367	40.565	1.00	10.33	A	O
ATOM	698	N	ASP	A	151	30.875	135.504	40.464	1.00	34.31	A	N
ATOM	699	CA	ASP	A	151	31.651	135.407	41.690	1.00	35.29	A	C
ATOM	700	CB	ASP	A	151	32.502	136.673	41.872	1.00	51.01	A	C
ATOM	701	CG	ASP	A	151	31.675	137.918	42.142	1.00	52.97	A	C
ATOM	702	OD1	ASP	A	151	30.759	138.219	41.349	1.00	52.30	A	O
ATOM	703	OD2	ASP	A	151	31.960	138.601	43.148	1.00	55.01	A	O
ATOM	704	C	ASP	A	151	30.757	135.161	42.912	1.00	37.14	A	C
ATOM	705	O	ASP	A	151	31.093	135.514	44.031	1.00	37.24	A	O
ATOM	706	N	GLY	A	152	29.606	134.554	42.690	1.00	36.51	A	N
ATOM	707	CA	GLY	A	152	28.727	134.265	43.797	1.00	37.54	A	C
ATOM	708	C	GLY	A	152	28.422	132.781	43.764	1.00	39.41	A	C
ATOM	709	O	GLY	A	152	28.031	132.182	44.765	1.00	40.69	A	O
ATOM	710	N	GLY	A	153	28.620	132.176	42.600	1.00	22.25	A	N
ATOM	711	CA	GLY	A	153	28.339	130.763	42.456	1.00	21.33	A	C
ATOM	712	C	GLY	A	153	26.857	130.538	42.656	1.00	21.83	A	C
ATOM	713	O	GLY	A	153	26.126	131.483	42.919	1.00	23.58	A	O
ATOM	714	N	SER	A	154	26.402	129.297	42.534	1.00	11.75	A	N
ATOM	715	CA	SER	A	154	24.981	129.007	42.705	1.00	11.50	A	C
ATOM	716	CB	SER	A	154	24.712	127.507	42.502	1.00	36.66	A	C
ATOM	717	OG	SER	A	154	25.553	126.685	43.294	1.00	39.60	A	O
ATOM	718	C	SER	A	154	24.464	129.450	44.065	1.00	9.74	A	C
ATOM	719	O	SER	A	154	25.233	129.575	45.020	1.00	8.80	A	O
ATOM	720	N	LEU	A	155	23.164	129.720	44.148	1.00	27.43	A	N
ATOM	721	CA	LEU	A	155	22.585	130.124	45.419	1.00	28.82	A	C
ATOM	722	CB	LEU	A	155	21.066	130.272	45.326	1.00	23.74	A	C
ATOM	723	CG	LEU	A	155	20.481	131.485	44.615	1.00	25.19	A	C
ATOM	724	CD1	LEU	A	155	18.989	131.496	44.835	1.00	24.64	A	C
ATOM	725	CD2	LEU	A	155	21.096	132.756	45.156	1.00	25.58	A	C

ATOM	726	C	LEU	A	155	22.920	128.965	46.321	1.00	29.95	A	C
ATOM	727	O	LEU	A	155	23.214	129.123	47.500	1.00	31.14	A	O
ATOM	728	N	ASP	A	156	22.868	127.786	45.729	1.00	29.30	A	N
ATOM	729	CA	ASP	A	156	23.184	126.562	46.424	1.00	26.79	A	C
ATOM	730	CB	ASP	A	156	23.394	125.452	45.402	1.00	80.89	A	C
ATOM	731	CG	ASP	A	156	23.083	124.091	45.954	1.00	82.14	A	C
ATOM	732	OD1	ASP	A	156	21.923	123.872	46.369	1.00	83.33	A	O
ATOM	733	OD2	ASP	A	156	23.997	123.242	45.966	1.00	82.60	A	O
ATOM	734	C	ASP	A	156	24.468	126.795	47.209	1.00	24.70	A	C
ATOM	735	O	ASP	A	156	24.575	126.407	48.364	1.00	25.77	A	O
ATOM	736	N	GLN	A	157	25.437	127.448	46.575	1.00	25.35	A	N
ATOM	737	CA	GLN	A	157	26.719	127.732	47.216	1.00	26.58	A	C
ATOM	738	CB	GLN	A	157	27.704	128.360	46.235	1.00	65.71	A	C
ATOM	739	CG	GLN	A	157	27.864	127.674	44.903	1.00	68.13	A	C
ATOM	740	CD	GLN	A	157	28.912	128.371	44.059	1.00	70.33	A	C
ATOM	741	OE1	GLN	A	157	29.083	128.079	42.873	1.00	72.22	A	O
ATOM	742	NE2	GLN	A	157	29.627	129.308	44.674	1.00	71.85	A	N
ATOM	743	C	GLN	A	157	26.517	128.716	48.346	1.00	25.10	A	C
ATOM	744	O	GLN	A	157	27.184	128.646	49.372	1.00	23.67	A	O
ATOM	745	N	VAL	A	158	25.610	129.655	48.124	1.00	25.08	A	N
ATOM	746	CA	VAL	A	158	25.302	130.671	49.106	1.00	25.32	A	C
ATOM	747	CB	VAL	A	158	24.388	131.757	48.491	1.00	48.72	A	C
ATOM	748	CG1	VAL	A	158	24.121	132.861	49.498	1.00	48.90	A	C
ATOM	749	CG2	VAL	A	158	25.034	132.334	47.262	1.00	47.90	A	C
ATOM	750	C	VAL	A	158	24.602	130.040	50.305	1.00	24.29	A	C
ATOM	751	O	VAL	A	158	24.760	130.489	51.437	1.00	23.32	A	O
ATOM	752	N	LEU	A	159	23.831	128.989	50.064	1.00	43.47	A	N
ATOM	753	CA	LEU	A	159	23.114	128.350	51.152	1.00	43.91	A	C
ATOM	754	CB	LEU	A	159	22.072	127.378	50.595	1.00	30.29	A	C
ATOM	755	CG	LEU	A	159	21.140	126.769	51.647	1.00	28.44	A	C
ATOM	756	CD1	LEU	A	159	20.667	127.870	52.554	1.00	27.40	A	C
ATOM	757	CD2	LEU	A	159	19.951	126.070	50.996	1.00	28.92	A	C
ATOM	758	C	LEU	A	159	24.048	127.636	52.126	1.00	43.36	A	C
ATOM	759	O	LEU	A	159	23.783	127.595	53.331	1.00	43.94	A	O
ATOM	760	N	LYS	A	160	25.141	127.078	51.612	1.00	44.16	A	N
ATOM	761	CA	LYS	A	160	26.079	126.384	52.477	1.00	46.53	A	C
ATOM	762	CB	LYS	A	160	27.265	125.838	51.685	1.00	65.55	A	C
ATOM	763	CG	LYS	A	160	28.449	125.465	52.589	1.00	67.52	A	C
ATOM	764	CD	LYS	A	160	29.568	124.730	51.845	1.00	69.50	A	C
ATOM	765	CE	LYS	A	160	30.773	124.428	52.754	1.00	69.72	A	C
ATOM	766	NZ	LYS	A	160	31.568	125.634	53.141	1.00	71.96	A	N
ATOM	767	C	LYS	A	160	26.590	127.325	53.554	1.00	48.43	A	C
ATOM	768	O	LYS	A	160	26.681	126.955	54.730	1.00	47.87	A	O

ATOM	769	N	GLU	A	161	26.917	128.547	53.144	1.00 61.96	A	N
ATOM	770	CA	GLU	A	161	27.434	129.554	54.060	1.00 61.47	A	C
ATOM	771	CB	GLU	A	161	28.321	130.550	53.309	1.00101.57	A	C
ATOM	772	CG	GLU	A	161	29.768	130.131	53.175	1.00106.66	A	C
ATOM	773	CD	GLU	A	161	30.660	131.295	52.800	1.00109.89	A	C
ATOM	774	OE1	GLU	A	161	30.463	131.870	51.707	1.00111.30	A	O
ATOM	775	OE2	GLU	A	161	31.553	131.641	53.603	1.00110.99	A	O
ATOM	776	C	GLU	A	161	26.373	130.331	54.835	1.00 60.11	A	C
ATOM	777	O	GLU	A	161	26.645	130.838	55.924	1.00 59.94	A	O
ATOM	778	N	ALA	A	162	25.167	130.420	54.289	1.00 59.64	A	N
ATOM	779	CA	ALA	A	162	24.108	131.172	54.948	1.00 59.64	A	C
ATOM	780	CB	ALA	A	162	23.307	131.929	53.904	1.00 40.04	A	C
ATOM	781	C	ALA	A	162	23.171	130.346	55.833	1.00 58.18	A	C
ATOM	782	O	ALA	A	162	22.421	130.907	56.632	1.00 56.75	A	O
ATOM	783	N	LYS	A	163	23.220	129.023	55.695	1.00 68.51	A	N
ATOM	784	CA	LYS	A	163	22.368	128.134	56.479	1.00 67.86	A	C
ATOM	785	CB	LYS	A	163	22.351	128.564	57.941	1.00 75.09	A	C
ATOM	786	CG	LYS	A	163	23.718	128.507	58.594	1.00 76.89	A	C
ATOM	787	CD	LYS	A	163	24.352	127.137	58.402	1.00 79.53	A	C
ATOM	788	CE	LYS	A	163	25.786	127.120	58.896	1.00 78.29	A	C
ATOM	789	NZ	LYS	A	163	25.869	127.499	60.339	1.00 78.07	A	N
ATOM	790	C	LYS	A	163	20.965	128.162	55.908	1.00 66.82	A	C
ATOM	791	O	LYS	A	163	20.546	127.221	55.239	1.00 66.92	A	O
ATOM	792	N	ARG	A	164	20.231	129.230	56.196	1.00 42.34	A	N
ATOM	793	CA	ARG	A	164	18.891	129.401	55.645	1.00 39.65	A	C
ATOM	794	CB	ARG	A	164	17.804	128.994	56.662	1.00120.19	A	C
ATOM	795	CG	ARG	A	164	17.947	129.507	58.091	1.00124.58	A	C
ATOM	796	CD	ARG	A	164	17.352	130.899	58.293	1.00125.42	A	C
ATOM	797	NE	ARG	A	164	18.271	131.970	57.903	1.00126.82	A	N
ATOM	798	CZ	ARG	A	164	18.025	133.271	58.051	1.00126.66	A	C
ATOM	799	NH1	ARG	A	164	16.883	133.682	58.586	1.00126.27	A	N
ATOM	800	NH2	ARG	A	164	18.925	134.165	57.666	1.00126.02	A	N
ATOM	801	C	ARG	A	164	18.741	130.857	55.170	1.00 35.62	A	C
ATOM	802	O	ARG	A	164	19.320	131.769	55.747	1.00 37.58	A	O
ATOM	803	N	ILE	A	165	17.994	131.072	54.096	1.00 40.22	A	N
ATOM	804	CA	ILE	A	165	17.837	132.412	53.562	1.00 35.51	A	C
ATOM	805	CB	ILE	A	165	17.655	132.379	52.049	1.00 13.61	A	C
ATOM	806	CG2	ILE	A	165	17.946	133.729	51.473	1.00 13.20	A	C
ATOM	807	CG1	ILE	A	165	18.623	131.388	51.415	1.00 13.20	A	C
ATOM	808	CD1	ILE	A	165	19.699	132.028	50.572	1.00 13.20	A	C
ATOM	809	C	ILE	A	165	16.656	133.165	54.144	1.00 34.51	A	C
ATOM	810	O	ILE	A	165	15.643	132.577	54.514	1.00 34.51	A	O
ATOM	811	N	PRO	A	166	16.784	134.489	54.253	1.00 15.61	A	N

ATOM	812	CD	PRO	A	166	18.098	135.154	54.281	1.00	32.45	A	C
ATOM	813	CA	PRO	A	166	15.746	135.376	54.775	1.00	16.93	A	C
ATOM	814	CB	PRO	A	166	16.498	136.680	54.991	1.00	32.16	A	C
ATOM	815	CG	PRO	A	166	17.883	136.209	55.318	1.00	32.44	A	C
ATOM	816	C	PRO	A	166	14.659	135.507	53.714	1.00	18.32	A	C
ATOM	817	O	PRO	A	166	14.965	135.703	52.550	1.00	21.03	A	O
ATOM	818	N	GLU	A	167	13.393	135.399	54.107	1.00	29.02	A	N
ATOM	819	CA	GLU	A	167	12.295	135.488	53.147	1.00	28.65	A	C
ATOM	820	CB	GLU	A	167	10.949	135.377	53.861	1.00	20.33	A	C
ATOM	821	CG	GLU	A	167	10.120	136.607	53.680	1.00	20.50	A	C
ATOM	822	CD	GLU	A	167	8.636	136.350	53.752	1.00	20.68	A	C
ATOM	823	OE1	GLU	A	167	8.144	135.832	54.774	1.00	23.43	A	O
ATOM	824	OE2	GLU	A	167	7.952	136.683	52.773	1.00	21.54	A	O
ATOM	825	C	GLU	A	167	12.290	136.738	52.254	1.00	29.27	A	C
ATOM	826	O	GLU	A	167	11.751	136.711	51.157	1.00	28.66	A	O
ATOM	827	N	GLU	A	168	12.882	137.833	52.710	1.00	35.90	A	N
ATOM	828	CA	GLU	A	168	12.907	139.030	51.888	1.00	38.87	A	C
ATOM	829	CB	GLU	A	168	13.045	140.276	52.755	1.00	82.82	A	C
ATOM	830	CG	GLU	A	168	11.702	140.772	53.240	1.00	91.11	A	C
ATOM	831	CD	GLU	A	168	10.698	140.927	52.100	1.00	96.97	A	C
ATOM	832	OE1	GLU	A	168	10.930	141.769	51.206	1.00	100.74	A	O
ATOM	833	OE2	GLU	A	168	9.677	140.204	52.094	1.00	101.06	A	O
ATOM	834	C	GLU	A	168	14.007	138.981	50.843	1.00	37.26	A	C
ATOM	835	O	GLU	A	168	13.999	139.743	49.882	1.00	38.57	A	O
ATOM	836	N	ILE	A	169	14.963	138.088	51.030	1.00	31.58	A	N
ATOM	837	CA	ILE	A	169	16.026	137.950	50.060	1.00	29.77	A	C
ATOM	838	CB	ILE	A	169	17.267	137.270	50.667	1.00	23.39	A	C
ATOM	839	CG2	ILE	A	169	18.236	136.869	49.568	1.00	22.81	A	C
ATOM	840	CG1	ILE	A	169	17.946	138.217	51.650	1.00	22.59	A	C
ATOM	841	CD1	ILE	A	169	18.478	139.481	51.014	1.00	21.36	A	C
ATOM	842	C	ILE	A	169	15.440	137.053	48.988	1.00	29.29	A	C
ATOM	843	O	ILE	A	169	15.601	137.290	47.790	1.00	27.77	A	O
ATOM	844	N	LEU	A	170	14.734	136.024	49.431	1.00	31.09	A	N
ATOM	845	CA	LEU	A	170	14.136	135.101	48.502	1.00	32.10	A	C
ATOM	846	CB	LEU	A	170	13.477	133.939	49.249	1.00	44.67	A	C
ATOM	847	CG	LEU	A	170	14.481	133.050	49.992	1.00	45.28	A	C
ATOM	848	CD1	LEU	A	170	13.793	131.776	50.452	1.00	45.00	A	C
ATOM	849	CD2	LEU	A	170	15.662	132.733	49.074	1.00	43.53	A	C
ATOM	850	C	LEU	A	170	13.128	135.854	47.658	1.00	32.46	A	C
ATOM	851	O	LEU	A	170	12.742	135.406	46.575	1.00	34.64	A	O
ATOM	852	N	GLY	A	171	12.701	137.010	48.145	1.00	22.61	A	N
ATOM	853	CA	GLY	A	171	11.762	137.789	47.368	1.00	21.78	A	C
ATOM	854	C	GLY	A	171	12.509	138.338	46.165	1.00	21.41	A	C

ATOM	855	O	GLY	A	171	12.060	138.226	45.023	1.00	20.42	A	O
ATOM	856	N	LYS	A	172	13.674	138.923	46.419	1.00	45.53	A	N
ATOM	857	CA	LYS	A	172	14.458	139.491	45.344	1.00	45.84	A	C
ATOM	858	CB	LYS	A	172	15.681	140.222	45.893	1.00	54.88	A	C
ATOM	859	CG	LYS	A	172	15.971	141.519	45.154	1.00	57.22	A	C
ATOM	860	CD	LYS	A	172	17.153	142.260	45.759	1.00	59.59	A	C
ATOM	861	CE	LYS	A	172	17.093	143.774	45.477	1.00	59.34	A	C
ATOM	862	NZ	LYS	A	172	17.026	144.136	44.027	1.00	60.24	A	N
ATOM	863	C	LYS	A	172	14.862	138.338	44.454	1.00	45.25	A	C
ATOM	864	O	LYS	A	172	15.047	138.494	43.249	1.00	47.10	A	O
ATOM	865	N	VAL	A	173	14.987	137.164	45.045	1.00	40.54	A	N
ATOM	866	CA	VAL	A	173	15.338	136.008	44.253	1.00	40.09	A	C
ATOM	867	CB	VAL	A	173	15.758	134.839	45.132	1.00	43.09	A	C
ATOM	868	CG1	VAL	A	173	15.864	133.581	44.297	1.00	44.23	A	C
ATOM	869	CG2	VAL	A	173	17.087	135.153	45.780	1.00	43.99	A	C
ATOM	870	C	VAL	A	173	14.134	135.598	43.417	1.00	39.88	A	C
ATOM	871	O	VAL	A	173	14.253	135.378	42.208	1.00	39.58	A	O
ATOM	872	N	SER	A	174	12.972	135.516	44.064	1.00	31.51	A	N
ATOM	873	CA	SER	A	174	11.729	135.134	43.397	1.00	31.80	A	C
ATOM	874	CB	SER	A	174	10.605	134.995	44.418	1.00	27.06	A	C
ATOM	875	OG	SER	A	174	10.759	133.813	45.168	1.00	27.06	A	O
ATOM	876	C	SER	A	174	11.281	136.075	42.282	1.00	31.24	A	C
ATOM	877	O	SER	A	174	10.397	135.742	41.499	1.00	31.24	A	O
ATOM	878	N	ILE	A	175	11.884	137.252	42.210	1.00	33.25	A	N
ATOM	879	CA	ILE	A	175	11.531	138.199	41.161	1.00	33.25	A	C
ATOM	880	CB	ILE	A	175	11.750	139.658	41.616	1.00	30.01	A	C
ATOM	881	CG2	ILE	A	175	11.686	140.594	40.433	1.00	29.51	A	C
ATOM	882	CG1	ILE	A	175	10.687	140.029	42.657	1.00	32.34	A	C
ATOM	883	CD1	ILE	A	175	10.988	141.274	43.440	1.00	34.32	A	C
ATOM	884	C	ILE	A	175	12.353	137.926	39.920	1.00	33.35	A	C
ATOM	885	O	ILE	A	175	11.809	137.873	38.833	1.00	33.25	A	O
ATOM	886	N	ALA	A	176	13.656	137.725	40.083	1.00	25.63	A	N
ATOM	887	CA	ALA	A	176	14.529	137.462	38.946	1.00	25.52	A	C
ATOM	888	CB	ALA	A	176	15.950	137.562	39.367	1.00	4.67	A	C
ATOM	889	C	ALA	A	176	14.285	136.106	38.300	1.00	25.52	A	C
ATOM	890	O	ALA	A	176	14.431	135.955	37.084	1.00	25.52	A	O
ATOM	891	N	VAL	A	177	13.937	135.108	39.104	1.00	27.76	A	N
ATOM	892	CA	VAL	A	177	13.664	133.781	38.566	1.00	27.76	A	C
ATOM	893	CB	VAL	A	177	13.309	132.808	39.674	1.00	18.77	A	C
ATOM	894	CG1	VAL	A	177	13.028	131.423	39.085	1.00	18.77	A	C
ATOM	895	CG2	VAL	A	177	14.428	132.789	40.694	1.00	18.77	A	C
ATOM	896	C	VAL	A	177	12.452	133.919	37.676	1.00	27.76	A	C
ATOM	897	O	VAL	A	177	12.432	133.514	36.519	1.00	27.76	A	O

ATOM	898	N	LEU	A	178	11.429	134.516	38.252	1.00	24.57	A	N
ATOM	899	CA	LEU	A	178	10.186	134.744	37.563	1.00	25.93	A	C
ATOM	900	CB	LEU	A	178	9.193	135.303	38.572	1.00	12.91	A	C
ATOM	901	CG	LEU	A	178	7.717	135.014	38.423	1.00	13.83	A	C
ATOM	902	CD1	LEU	A	178	7.463	133.562	38.700	1.00	12.38	A	C
ATOM	903	CD2	LEU	A	178	6.966	135.905	39.390	1.00	14.17	A	C
ATOM	904	C	LEU	A	178	10.370	135.708	36.375	1.00	26.02	A	C
ATOM	905	O	LEU	A	178	9.556	135.753	35.474	1.00	26.84	A	O
ATOM	906	N	ARG	A	179	11.432	136.489	36.361	1.00	27.42	A	N
ATOM	907	CA	ARG	A	179	11.615	137.388	35.239	1.00	29.12	A	C
ATOM	908	CB	ARG	A	179	12.175	138.727	35.701	1.00	29.61	A	C
ATOM	909	CG	ARG	A	179	11.144	139.544	36.434	1.00	32.74	A	C
ATOM	910	CD	ARG	A	179	11.592	140.957	36.683	1.00	36.42	A	C
ATOM	911	NE	ARG	A	179	10.706	141.614	37.633	1.00	40.58	A	N
ATOM	912	CZ	ARG	A	179	10.893	142.843	38.092	1.00	42.89	A	C
ATOM	913	NH1	ARG	A	179	10.043	143.367	38.963	1.00	45.42	A	N
ATOM	914	NH2	ARG	A	179	11.929	143.549	37.672	1.00	42.71	A	N
ATOM	915	C	ARG	A	179	12.517	136.776	34.193	1.00	28.23	A	C
ATOM	916	O	ARG	A	179	12.365	137.036	32.998	1.00	29.46	A	O
ATOM	917	N	GLY	A	180	13.465	135.964	34.641	1.00	36.88	A	N
ATOM	918	CA	GLY	A	180	14.354	135.309	33.706	1.00	36.46	A	C
ATOM	919	C	GLY	A	180	13.567	134.240	32.979	1.00	35.03	A	C
ATOM	920	O	GLY	A	180	13.678	134.084	31.772	1.00	34.75	A	O
ATOM	921	N	LEU	A	181	12.756	133.511	33.732	1.00	20.70	A	N
ATOM	922	CA	LEU	A	181	11.937	132.455	33.176	1.00	21.10	A	C
ATOM	923	CB	LEU	A	181	11.052	131.854	34.272	1.00	4.67	A	C
ATOM	924	CG	LEU	A	181	11.146	130.337	34.459	1.00	5.06	A	C
ATOM	925	CD1	LEU	A	181	12.542	129.865	34.137	1.00	5.95	A	C
ATOM	926	CD2	LEU	A	181	10.776	129.979	35.873	1.00	4.67	A	C
ATOM	927	C	LEU	A	181	11.074	133.073	32.095	1.00	20.95	A	C
ATOM	928	O	LEU	A	181	10.987	132.579	30.962	1.00	21.25	A	O
ATOM	929	N	ALA	A	182	10.449	134.180	32.462	1.00	45.47	A	N
ATOM	930	CA	ALA	A	182	9.569	134.908	31.571	1.00	46.06	A	C
ATOM	931	CB	ALA	A	182	8.958	136.034	32.325	1.00	4.67	A	C
ATOM	932	C	ALA	A	182	10.268	135.435	30.315	1.00	45.46	A	C
ATOM	933	O	ALA	A	182	9.745	135.300	29.211	1.00	46.13	A	O
ATOM	934	N	TYR	A	183	11.437	136.043	30.495	1.00	27.66	A	N
ATOM	935	CA	TYR	A	183	12.212	136.596	29.397	1.00	29.18	A	C
ATOM	936	CB	TYR	A	183	13.526	137.131	29.922	1.00	34.60	A	C
ATOM	937	CG	TYR	A	183	14.444	137.623	28.833	1.00	34.56	A	C
ATOM	938	CD1	TYR	A	183	14.267	138.878	28.267	1.00	34.56	A	C
ATOM	939	CE1	TYR	A	183	15.092	139.330	27.267	1.00	34.95	A	C
ATOM	940	CD2	TYR	A	183	15.482	136.828	28.361	1.00	34.56	A	C

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ATOM    941  CE2 TYR A 183     16.310 137.270  27.355  1.00 35.13      A    C
ATOM    942  CZ  TYR A 183     16.108 138.524  26.808  1.00 35.69      A    C
ATOM    943  OH  TYR A 183     16.889 138.967  25.765  1.00 38.39      A    O
ATOM    944  C   TYR A 183     12.499 135.536  28.347  1.00 27.78      A    C
ATOM    945  O   TYR A 183     12.407 135.786  27.151  1.00 30.13      A    O
ATOM    946  N   LEU A 184     12.884 134.355  28.795  1.00  5.40      A    N
ATOM    947  CA  LEU A 184     13.149 133.280  27.874  1.00  6.16      A    C
ATOM    948  CB  LEU A 184     13.707 132.086  28.609  1.00 13.95      A    C
ATOM    949  CG  LEU A 184     14.985 132.444  29.342  1.00 13.50      A    C
ATOM    950  CD1 LEU A 184     15.496 131.216  30.031  1.00 13.24      A    C
ATOM    951  CD2 LEU A 184     16.014 132.987  28.374  1.00 14.33      A    C
ATOM    952  C   LEU A 184     11.856 132.888  27.213  1.00  9.15      A    C
ATOM    953  O   LEU A 184     11.805 132.709  26.011  1.00  8.33      A    O
ATOM    954  N   ARG A 185     10.789 132.750  28.017  1.00 13.27      A    N
ATOM    955  CA  ARG A 185      9.497 132.368  27.464  1.00 18.44      A    C
ATOM    956  CB  ARG A 185      8.400 132.366  28.530  1.00 13.15      A    C
ATOM    957  CG  ARG A 185      7.535 131.117  28.379  1.00 17.39      A    C
ATOM    958  CD  ARG A 185      6.026 131.311  28.499  1.00 20.29      A    C
ATOM    959  NE  ARG A 185      5.341 130.105  28.030  1.00 26.10      A    N
ATOM    960  CZ  ARG A 185      4.025 129.938  28.009  1.00 29.27      A    C
ATOM    961  NH1 ARG A 185      3.221 130.898  28.439  1.00 32.97      A    N
ATOM    962  NH2 ARG A 185      3.510 128.814  27.538  1.00 30.75      A    N
ATOM    963  C   ARG A 185      9.125 133.300  26.346  1.00 20.19      A    C
ATOM    964  O   ARG A 185      9.344 133.004  25.182  1.00 20.65      A    O
ATOM    965  N   GLU A 186      8.598 134.474  26.722  1.00 29.26      A    N
ATOM    966  CA  GLU A 186      8.156 135.497  25.784  1.00 31.82      A    C
ATOM    967  CB  GLU A 186      7.837 136.764  26.561  1.00 50.08      A    C
ATOM    968  CG  GLU A 186      6.746 136.569  27.605  1.00 49.00      A    C
ATOM    969  CD  GLU A 186      6.774 137.639  28.668  1.00 47.82      A    C
ATOM    970  OE1 GLU A 186      6.184 137.428  29.747  1.00 48.06      A    O
ATOM    971  OE2 GLU A 186      7.396 138.693  28.416  1.00 47.27      A    O
ATOM    972  C   GLU A 186      9.035 135.831  24.588  1.00 33.17      A    C
ATOM    973  O   GLU A 186      8.641 135.597  23.446  1.00 35.08      A    O
ATOM    974  N   LYS A 187     10.226 136.367  24.834  1.00 37.34      A    N
ATOM    975  CA  LYS A 187     11.108 136.754  23.737  1.00 37.86      A    C
ATOM    976  CB  LYS A 187     12.271 137.563  24.294  1.00 80.48      A    C
ATOM    977  CG  LYS A 187     11.812 138.822  24.997  1.00 83.34      A    C
ATOM    978  CD  LYS A 187     11.035 139.722  24.055  1.00 85.98      A    C
ATOM    979  CE  LYS A 187     10.581 140.985  24.749  1.00 87.49      A    C
ATOM    980  NZ  LYS A 187     10.148 141.982  23.737  1.00 90.60      A    N
ATOM    981  C   LYS A 187     11.646 135.650  22.848  1.00 37.53      A    C
ATOM    982  O   LYS A 187     11.386 135.630  21.648  1.00 38.18      A    O
ATOM    983  N   HIS A 188     12.387 134.733  23.441  1.00 34.96      A    N
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ATOM    984  CA  HIS A 188     12.984 133.615  22.727  1.00 34.41      A    C
ATOM    985  CB  HIS A 188     14.340 133.336  23.320  1.00 59.70      A    C
ATOM    986  CG  HIS A 188     15.252 134.506  23.295  1.00 56.86      A    C
ATOM    987  CD2 HIS A 188     15.446 135.504  24.183  1.00 54.78      A    C
ATOM    988  ND1 HIS A 188     16.109 134.743  22.251  1.00 56.23      A    N
ATOM    989  CE1 HIS A 188     16.805 135.835  22.497  1.00 55.39      A    C
ATOM    990  NE2 HIS A 188     16.424 136.314  23.666  1.00 53.27      A    N
ATOM    991  C   HIS A 188     12.231 132.288  22.726  1.00 35.80      A    C
ATOM    992  O   HIS A 188     12.838 131.263  22.444  1.00 36.43      A    O
ATOM    993  N   GLN A 189     10.946 132.261  23.040  1.00 38.19      A    N
ATOM    994  CA  GLN A 189     10.240 130.978  23.089  1.00 40.76      A    C
ATOM    995  CB  GLN A 189      9.601 130.656  21.733  1.00 60.17      A    C
ATOM    996  CG  GLN A 189      8.630 131.710  21.259  1.00 64.35      A    C
ATOM    997  CD  GLN A 189      9.326 132.854  20.550  1.00 68.11      A    C
ATOM    998  OE1 GLN A 189      8.772 133.949  20.415  1.00 69.02      A    O
ATOM    999  NE2 GLN A 189     10.543 132.601  20.075  1.00 69.63      A    N
ATOM   1000  C   GLN A 189     11.126 129.792  23.540  1.00 40.91      A    C
ATOM   1001  O   GLN A 189     11.501 128.931  22.739  1.00 41.24      A    O
ATOM   1002  N   ILE A 190     11.462 129.748  24.825  1.00 35.51      A    N
ATOM   1003  CA  ILE A 190     12.263 128.655  25.336  1.00 33.88      A    C
ATOM   1004  CB  ILE A 190     13.753 128.886  25.034  1.00 62.27      A    C
ATOM   1005  CG2 ILE A 190     14.479 129.370  26.266  1.00 63.56      A    C
ATOM   1006  CG1 ILE A 190     14.369 127.579  24.540  1.00 63.51      A    C
ATOM   1007  CD1 ILE A 190     13.614 126.955  23.364  1.00 65.10      A    C
ATOM   1008  C   ILE A 190     12.036 128.480  26.831  1.00 30.65      A    C
ATOM   1009  O   ILE A 190     11.993 129.464  27.568  1.00 29.37      A    O
ATOM   1010  N   MET A 191     11.869 127.225  27.264  1.00 28.95      A    N
ATOM   1011  CA  MET A 191     11.637 126.890  28.676  1.00 27.94      A    C
ATOM   1012  CB  MET A 191     10.675 125.719  28.801  1.00 21.84      A    C
ATOM   1013  CG  MET A 191      9.630 125.682  27.724  1.00 26.83      A    C
ATOM   1014  SD  MET A 191      8.703 124.186  27.853  1.00 34.46      A    S
ATOM   1015  CE  MET A 191      7.045 124.782  27.588  1.00 32.21      A    C
ATOM   1016  C   MET A 191     12.954 126.512  29.316  1.00 25.43      A    C
ATOM   1017  O   MET A 191     13.941 126.285  28.624  1.00 24.34      A    O
ATOM   1018  N   HIS A 192     12.963 126.406  30.637  1.00 26.76      A    N
ATOM   1019  CA  HIS A 192     14.199 126.104  31.351  1.00 25.38      A    C
ATOM   1020  CB  HIS A 192     14.115 126.625  32.778  1.00 32.34      A    C
ATOM   1021  CG  HIS A 192     15.439 126.990  33.339  1.00 29.31      A    C
ATOM   1022  CD2 HIS A 192     15.952 128.185  33.707  1.00 29.50      A    C
ATOM   1023  ND1 HIS A 192     16.456 126.076  33.477  1.00 27.51      A    N
ATOM   1024  CE1 HIS A 192     17.544 126.692  33.903  1.00 28.37      A    C
ATOM   1025  NE2 HIS A 192     17.265 127.974  34.049  1.00 29.05      A    N
ATOM   1026  C   HIS A 192     14.633 124.648  31.397  1.00 24.77      A    C
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ATOM	1027	O	HIS A 192	15.797	124.324	31.147	1.00	26.08	A	O
ATOM	1028	N	ARG A 193	13.700	123.775	31.745	1.00	34.20	A	N
ATOM	1029	CA	ARG A 193	13.989	122.363	31.833	1.00	35.28	A	C
ATOM	1030	CB	ARG A 193	14.518	121.862	30.496	1.00	45.77	A	C
ATOM	1031	CG	ARG A 193	13.800	122.409	29.291	1.00	48.75	A	C
ATOM	1032	CD	ARG A 193	14.200	121.610	28.067	1.00	51.24	A	C
ATOM	1033	NE	ARG A 193	13.342	120.443	27.869	1.00	55.34	A	N
ATOM	1034	CZ	ARG A 193	12.181	120.470	27.218	1.00	56.23	A	C
ATOM	1035	NH1	ARG A 193	11.726	121.603	26.692	1.00	55.68	A	N
ATOM	1036	NH2	ARG A 193	11.474	119.358	27.086	1.00	56.63	A	N
ATOM	1037	C	ARG A 193	15.005	122.050	32.929	1.00	36.38	A	C
ATOM	1038	O	ARG A 193	15.453	120.912	33.050	1.00	37.15	A	O
ATOM	1039	N	ASP A 194	15.376	123.042	33.730	1.00	31.52	A	N
ATOM	1040	CA	ASP A 194	16.348	122.790	34.787	1.00	30.05	A	C
ATOM	1041	CB	ASP A 194	17.714	122.498	34.155	1.00	34.62	A	C
ATOM	1042	CG	ASP A 194	18.620	121.672	35.059	1.00	35.80	A	C
ATOM	1043	OD1	ASP A 194	18.091	120.912	35.898	1.00	36.47	A	O
ATOM	1044	OD2	ASP A 194	19.862	121.758	34.916	1.00	38.05	A	O
ATOM	1045	C	ASP A 194	16.464	123.915	35.820	1.00	28.41	A	C
ATOM	1046	O	ASP A 194	17.543	124.455	36.049	1.00	26.95	A	O
ATOM	1047	N	VAL A 195	15.344	124.253	36.448	1.00	26.14	A	N
ATOM	1048	CA	VAL A 195	15.334	125.290	37.469	1.00	26.17	A	C
ATOM	1049	CB	VAL A 195	13.959	125.938	37.616	1.00	20.94	A	C
ATOM	1050	CG1	VAL A 195	13.941	126.779	38.863	1.00	21.72	A	C
ATOM	1051	CG2	VAL A 195	13.629	126.766	36.382	1.00	20.51	A	C
ATOM	1052	C	VAL A 195	15.663	124.675	38.810	1.00	25.35	A	C
ATOM	1053	O	VAL A 195	14.898	123.890	39.342	1.00	25.80	A	O
ATOM	1054	N	LYS A 196	16.809	125.019	39.359	1.00	17.39	A	N
ATOM	1055	CA	LYS A 196	17.194	124.486	40.648	1.00	17.56	A	C
ATOM	1056	CB	LYS A 196	17.758	123.068	40.503	1.00	73.82	A	C
ATOM	1057	CG	LYS A 196	18.672	122.873	39.309	1.00	75.77	A	C
ATOM	1058	CD	LYS A 196	19.319	121.495	39.298	1.00	79.13	A	C
ATOM	1059	CE	LYS A 196	20.247	121.316	40.489	1.00	82.20	A	C
ATOM	1060	NZ	LYS A 196	21.157	120.137	40.354	1.00	83.24	A	N
ATOM	1061	C	LYS A 196	18.221	125.412	41.253	1.00	17.05	A	C
ATOM	1062	O	LYS A 196	18.966	126.092	40.544	1.00	17.83	A	O
ATOM	1063	N	PRO A 197	18.259	125.472	42.579	1.00	33.46	A	N
ATOM	1064	CD	PRO A 197	17.391	124.688	43.473	1.00	14.08	A	C
ATOM	1065	CA	PRO A 197	19.185	126.311	43.338	1.00	33.48	A	C
ATOM	1066	CB	PRO A 197	19.196	125.637	44.692	1.00	14.99	A	C
ATOM	1067	CG	PRO A 197	17.743	125.242	44.833	1.00	14.47	A	C
ATOM	1068	C	PRO A 197	20.592	126.489	42.753	1.00	34.35	A	C
ATOM	1069	O	PRO A 197	21.173	127.569	42.865	1.00	33.04	A	O

ATOM	1070	N	SER	A	198	21.147	125.453	42.128	1.00	43.42	A	N
ATOM	1071	CA	SER	A	198	22.495	125.571	41.561	1.00	43.01	A	C
ATOM	1072	CB	SER	A	198	23.173	124.210	41.520	1.00	46.08	A	C
ATOM	1073	OG	SER	A	198	22.368	123.279	40.824	1.00	45.86	A	O
ATOM	1074	C	SER	A	198	22.575	126.193	40.173	1.00	44.56	A	C
ATOM	1075	O	SER	A	198	23.667	126.364	39.633	1.00	44.78	A	O
ATOM	1076	N	ASN	A	199	21.430	126.520	39.588	1.00	20.07	A	N
ATOM	1077	CA	ASN	A	199	21.416	127.110	38.266	1.00	21.65	A	C
ATOM	1078	CB	ASN	A	199	20.511	126.322	37.317	1.00	21.22	A	C
ATOM	1079	CG	ASN	A	199	21.096	124.966	36.925	1.00	23.57	A	C
ATOM	1080	OD1	ASN	A	199	22.309	124.819	36.745	1.00	26.70	A	O
ATOM	1081	ND2	ASN	A	199	20.225	123.975	36.770	1.00	25.53	A	N
ATOM	1082	C	ASN	A	199	20.938	128.538	38.379	1.00	22.16	A	C
ATOM	1083	O	ASN	A	199	20.622	129.187	37.380	1.00	21.91	A	O
ATOM	1084	N	ILE	A	200	20.879	129.008	39.621	1.00	20.03	A	N
ATOM	1085	CA	ILE	A	200	20.488	130.379	39.956	1.00	20.69	A	C
ATOM	1086	CB	ILE	A	200	19.402	130.398	41.049	1.00	12.72	A	C
ATOM	1087	CG2	ILE	A	200	19.171	131.814	41.517	1.00	13.96	A	C
ATOM	1088	CG1	ILE	A	200	18.123	129.727	40.517	1.00	10.59	A	C
ATOM	1089	CD1	ILE	A	200	16.972	129.731	41.469	1.00	7.37	A	C
ATOM	1090	C	ILE	A	200	21.772	130.968	40.504	1.00	23.72	A	C
ATOM	1091	O	ILE	A	200	22.155	130.686	41.628	1.00	24.27	A	O
ATOM	1092	N	LEU	A	201	22.449	131.774	39.700	1.00	22.45	A	N
ATOM	1093	CA	LEU	A	201	23.727	132.344	40.104	1.00	25.85	A	C
ATOM	1094	CB	LEU	A	201	24.706	132.238	38.936	1.00	29.40	A	C
ATOM	1095	CG	LEU	A	201	24.622	130.918	38.168	1.00	29.13	A	C
ATOM	1096	CD1	LEU	A	201	25.667	130.888	37.078	1.00	26.41	A	C
ATOM	1097	CD2	LEU	A	201	24.817	129.757	39.133	1.00	30.35	A	C
ATOM	1098	C	LEU	A	201	23.691	133.781	40.606	1.00	28.48	A	C
ATOM	1099	O	LEU	A	201	22.860	134.584	40.180	1.00	29.08	A	O
ATOM	1100	N	VAL	A	202	24.615	134.098	41.511	1.00	28.12	A	N
ATOM	1101	CA	VAL	A	202	24.719	135.440	42.082	1.00	31.97	A	C
ATOM	1102	CB	VAL	A	202	24.361	135.430	43.586	1.00	31.68	A	C
ATOM	1103	CG1	VAL	A	202	22.873	135.169	43.761	1.00	33.20	A	C
ATOM	1104	CG2	VAL	A	202	25.159	134.362	44.307	1.00	32.69	A	C
ATOM	1105	C	VAL	A	202	26.125	136.015	41.892	1.00	34.69	A	C
ATOM	1106	O	VAL	A	202	27.045	135.298	41.506	1.00	34.81	A	O
ATOM	1107	N	ASN	A	203	26.290	137.308	42.153	1.00	54.40	A	N
ATOM	1108	CA	ASN	A	203	27.598	137.941	41.984	1.00	55.96	A	C
ATOM	1109	CB	ASN	A	203	27.723	138.510	40.560	1.00	35.71	A	C
ATOM	1110	CG	ASN	A	203	26.766	139.653	40.306	1.00	37.27	A	C
ATOM	1111	OD1	ASN	A	203	25.829	139.856	41.068	1.00	38.58	A	O
ATOM	1112	ND2	ASN	A	203	26.990	140.399	39.232	1.00	37.90	A	N

ATOM	1113	C	ASN A 203	27.835	139.041	43.018	1.00	56.35	A	C
ATOM	1114	O	ASN A 203	26.912	139.437	43.723	1.00	56.23	A	O
ATOM	1115	N	SER A 204	29.079	139.518	43.105	1.00	59.50	A	N
ATOM	1116	CA	SER A 204	29.454	140.568	44.056	1.00	58.93	A	C
ATOM	1117	CB	SER A 204	30.905	140.990	43.835	1.00	67.61	A	C
ATOM	1118	OG	SER A 204	31.219	141.001	42.455	1.00	67.29	A	O
ATOM	1119	C	SER A 204	28.532	141.765	43.926	1.00	58.45	A	C
ATOM	1120	O	SER A 204	28.438	142.599	44.824	1.00	59.03	A	O
ATOM	1121	N	ARG A 205	27.868	141.850	42.783	1.00	60.64	A	N
ATOM	1122	CA	ARG A 205	26.903	142.901	42.537	1.00	61.13	A	C
ATOM	1123	CB	ARG A 205	26.868	143.250	41.052	1.00	176.25	A	C
ATOM	1124	CG	ARG A 205	28.089	144.025	40.582	1.00	180.43	A	C
ATOM	1125	CD	ARG A 205	29.393	143.237	40.723	1.00	183.79	A	C
ATOM	1126	NE	ARG A 205	29.728	142.478	39.518	1.00	187.06	A	N
ATOM	1127	CZ	ARG A 205	30.927	141.957	39.269	1.00	189.56	A	C
ATOM	1128	NH1	ARG A 205	31.140	141.284	38.145	1.00	190.69	A	N
ATOM	1129	NH2	ARG A 205	31.919	142.112	40.139	1.00	190.32	A	N
ATOM	1130	C	ARG A 205	25.601	142.235	42.977	1.00	59.58	A	C
ATOM	1131	O	ARG A 205	25.514	141.011	43.006	1.00	59.00	A	O
ATOM	1132	N	GLY A 206	24.592	143.015	43.329	1.00	66.69	A	N
ATOM	1133	CA	GLY A 206	23.358	142.408	43.785	1.00	64.01	A	C
ATOM	1134	C	GLY A 206	22.616	141.584	42.753	1.00	62.84	A	C
ATOM	1135	O	GLY A 206	21.443	141.270	42.954	1.00	61.70	A	O
ATOM	1136	N	GLU A 207	23.292	141.215	41.666	1.00	51.62	A	N
ATOM	1137	CA	GLU A 207	22.676	140.448	40.579	1.00	49.29	A	C
ATOM	1138	CB	GLU A 207	23.543	140.553	39.331	1.00	22.37	A	C
ATOM	1139	CG	GLU A 207	23.451	141.847	38.568	1.00	24.17	A	C
ATOM	1140	CD	GLU A 207	24.274	141.779	37.291	1.00	24.97	A	C
ATOM	1141	OE1	GLU A 207	23.807	142.260	36.232	1.00	25.21	A	O
ATOM	1142	OE2	GLU A 207	25.402	141.233	37.342	1.00	24.95	A	O
ATOM	1143	C	GLU A 207	22.328	138.967	40.822	1.00	48.14	A	C
ATOM	1144	O	GLU A 207	23.087	138.220	41.450	1.00	48.77	A	O
ATOM	1145	N	ILE A 208	21.168	138.563	40.298	1.00	24.86	A	N
ATOM	1146	CA	ILE A 208	20.666	137.196	40.416	1.00	23.35	A	C
ATOM	1147	CB	ILE A 208	19.426	137.129	41.303	1.00	9.53	A	C
ATOM	1148	CG2	ILE A 208	18.806	135.746	41.207	1.00	7.68	A	C
ATOM	1149	CG1	ILE A 208	19.791	137.497	42.742	1.00	10.23	A	C
ATOM	1150	CD1	ILE A 208	18.606	137.503	43.696	1.00	9.94	A	C
ATOM	1151	C	ILE A 208	20.264	136.717	39.038	1.00	22.99	A	C
ATOM	1152	O	ILE A 208	19.310	137.229	38.463	1.00	22.98	A	O
ATOM	1153	N	LYS A 209	20.973	135.721	38.518	1.00	48.95	A	N
ATOM	1154	CA	LYS A 209	20.685	135.224	37.182	1.00	48.19	A	C
ATOM	1155	CB	LYS A 209	21.861	135.535	36.272	1.00	54.62	A	C

ATOM	1156	CG	LYS A 209	22.279	136.980	36.387	1.00	56.31	A	C
ATOM	1157	CD	LYS A 209	23.327	137.379	35.386	1.00	60.80	A	C
ATOM	1158	CE	LYS A 209	23.582	138.864	35.500	1.00	64.03	A	C
ATOM	1159	NZ	LYS A 209	24.508	139.349	34.451	1.00	67.14	A	N
ATOM	1160	C	LYS A 209	20.337	133.754	37.052	1.00	47.24	A	C
ATOM	1161	O	LYS A 209	20.326	133.003	38.030	1.00	47.34	A	O
ATOM	1162	N	LEU A 210	20.034	133.362	35.819	1.00	47.33	A	N
ATOM	1163	CA	LEU A 210	19.688	131.991	35.483	1.00	45.09	A	C
ATOM	1164	CB	LEU A 210	18.359	131.941	34.737	1.00	21.98	A	C
ATOM	1165	CG	LEU A 210	17.055	132.245	35.474	1.00	21.89	A	C
ATOM	1166	CD1	LEU A 210	15.900	132.194	34.494	1.00	20.92	A	C
ATOM	1167	CD2	LEU A 210	16.833	131.232	36.573	1.00	21.60	A	C
ATOM	1168	C	LEU A 210	20.772	131.447	34.572	1.00	44.94	A	C
ATOM	1169	O	LEU A 210	21.731	132.148	34.246	1.00	46.12	A	O
ATOM	1170	N	CYS A 211	20.614	130.196	34.164	1.00	36.27	A	N
ATOM	1171	CA	CYS A 211	21.564	129.545	33.264	1.00	35.26	A	C
ATOM	1172	CB	CYS A 211	22.992	129.670	33.789	1.00	51.86	A	C
ATOM	1173	SG	CYS A 211	23.325	128.629	35.192	1.00	60.23	A	S
ATOM	1174	C	CYS A 211	21.215	128.075	33.076	1.00	33.37	A	C
ATOM	1175	O	CYS A 211	20.174	127.605	33.540	1.00	33.15	A	O
ATOM	1176	N	ASP A 212	22.109	127.359	32.408	1.00	53.41	A	N
ATOM	1177	CA	ASP A 212	21.904	125.946	32.095	1.00	53.22	A	C
ATOM	1178	CB	ASP A 212	22.194	125.061	33.317	1.00	54.27	A	C
ATOM	1179	CG	ASP A 212	23.648	125.149	33.780	1.00	59.13	A	C
ATOM	1180	OD1	ASP A 212	24.523	125.445	32.938	1.00	62.53	A	O
ATOM	1181	OD2	ASP A 212	23.925	124.907	34.975	1.00	57.75	A	O
ATOM	1182	C	ASP A 212	20.479	125.704	31.572	1.00	52.99	A	C
ATOM	1183	O	ASP A 212	19.910	124.637	31.794	1.00	52.65	A	O
ATOM	1184	N	PHE A 213	19.907	126.691	30.872	1.00	28.84	A	N
ATOM	1185	CA	PHE A 213	18.555	126.564	30.316	1.00	30.14	A	C
ATOM	1186	CB	PHE A 213	17.809	127.897	30.395	1.00	25.94	A	C
ATOM	1187	CG	PHE A 213	18.612	129.071	29.954	1.00	24.15	A	C
ATOM	1188	CD1	PHE A 213	18.535	129.526	28.657	1.00	22.83	A	C
ATOM	1189	CD2	PHE A 213	19.449	129.720	30.838	1.00	23.09	A	C
ATOM	1190	CE1	PHE A 213	19.263	130.608	28.250	1.00	22.72	A	C
ATOM	1191	CE2	PHE A 213	20.190	130.812	30.434	1.00	23.20	A	C
ATOM	1192	CZ	PHE A 213	20.093	131.257	29.134	1.00	23.97	A	C
ATOM	1193	C	PHE A 213	18.619	126.048	28.882	1.00	32.27	A	C
ATOM	1194	O	PHE A 213	19.516	126.407	28.127	1.00	35.09	A	O
ATOM	1195	N	GLY A 214	17.655	125.206	28.525	1.00	28.87	A	N
ATOM	1196	CA	GLY A 214	17.628	124.577	27.215	1.00	32.74	A	C
ATOM	1197	C	GLY A 214	17.458	125.391	25.958	1.00	35.13	A	C
ATOM	1198	O	GLY A 214	16.389	125.391	25.362	1.00	37.40	A	O

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ATOM   1199  N   VAL A 215     18.522 126.043  25.516  1.00 32.06      A    N
ATOM   1200  CA  VAL A 215     18.446 126.860  24.319  1.00 34.14      A    C
ATOM   1201  CB  VAL A 215     19.600 127.843  24.269  1.00 40.55      A    C
ATOM   1202  CG1 VAL A 215     19.743 128.513  25.611  1.00 40.57      A    C
ATOM   1203  CG2 VAL A 215     20.873 127.124  23.901  1.00 41.33      A    C
ATOM   1204  C   VAL A 215     18.446 126.066  23.022  1.00 36.13      A    C
ATOM   1205  O   VAL A 215     17.936 126.547  22.016  1.00 36.39      A    O
ATOM   1206  N   SER A 216     19.017 124.864  23.023  1.00 32.42      A    N
ATOM   1207  CA  SER A 216     19.045 124.060  21.802  1.00 35.47      A    C
ATOM   1208  CB  SER A 216     20.487 123.771  21.366  1.00 40.17      A    C
ATOM   1209  OG  SER A 216     21.159 122.956  22.303  1.00 41.17      A    O
ATOM   1210  C   SER A 216     18.286 122.747  21.920  1.00 36.65      A    C
ATOM   1211  O   SER A 216     18.586 121.907  22.771  1.00 36.42      A    O
ATOM   1212  N   GLY A 217     17.294 122.583  21.050  1.00135.31      A    N
ATOM   1213  CA  GLY A 217     16.499 121.372  21.048  1.00136.89      A    C
ATOM   1214  C   GLY A 217     17.383 120.164  20.825  1.00137.34      A    C
ATOM   1215  O   GLY A 217     16.969 119.029  21.059  1.00137.23      A    O
ATOM   1216  N   GLN A 218     18.605 120.408  20.364  1.00 36.49      A    N
ATOM   1217  CA  GLN A 218     19.540 119.327  20.128  1.00 38.71      A    C
ATOM   1218  CB  GLN A 218     20.583 119.708  19.071  1.00 67.45      A    C
ATOM   1219  CG  GLN A 218     20.365 119.025  17.712  1.00 67.78      A    C
ATOM   1220  CD  GLN A 218     20.269 117.501  17.820  1.00 69.08      A    C
ATOM   1221  OE1 GLN A 218     21.209 116.834  18.271  1.00 71.18      A    O
ATOM   1222  NE2 GLN A 218     19.128 116.947  17.409  1.00 68.45      A    N
ATOM   1223  C   GLN A 218     20.208 119.002  21.437  1.00 39.62      A    C
ATOM   1224  O   GLN A 218     19.791 118.076  22.110  1.00 39.34      A    O
ATOM   1225  N   LEU A 219     21.230 119.775  21.795  1.00 51.15      A    N
ATOM   1226  CA  LEU A 219     21.979 119.594  23.042  1.00 51.21      A    C
ATOM   1227  CB  LEU A 219     22.409 120.948  23.589  1.00 33.75      A    C
ATOM   1228  CG  LEU A 219     23.813 120.997  24.167  1.00 33.30      A    C
ATOM   1229  CD1 LEU A 219     24.014 122.313  24.879  1.00 31.59      A    C
ATOM   1230  CD2 LEU A 219     24.012 119.834  25.102  1.00 33.30      A    C
ATOM   1231  C   LEU A 219     21.149 118.877  24.099  1.00 54.40      A    C
ATOM   1232  O   LEU A 219     21.606 117.899  24.699  1.00 54.06      A    O
ATOM   1233  N   ILE A 220     19.941 119.386  24.338  1.00 35.07      A    N
ATOM   1234  CA  ILE A 220     19.027 118.770  25.291  1.00 34.36      A    C
ATOM   1235  CB  ILE A 220     17.596 119.339  25.167  1.00 35.67      A    C
ATOM   1236  CG2 ILE A 220     16.646 118.519  26.012  1.00 36.68      A    C
ATOM   1237  CG1 ILE A 220     17.553 120.805  25.598  1.00 35.98      A    C
ATOM   1238  CD1 ILE A 220     17.660 121.010  27.095  1.00 35.27      A    C
ATOM   1239  C   ILE A 220     18.974 117.323  24.842  1.00 36.39      A    C
ATOM   1240  O   ILE A 220     19.608 116.446  25.429  1.00 37.33      A    O
ATOM   1241  N   ASP A 221     18.230 117.113  23.760  1.00 49.00      A    N
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ATOM	1242	CA	ASP	A	221	18.032	115.813	23.132	1.00 50.55	A	C
ATOM	1243	CB	ASP	A	221	17.529	116.026	21.701	1.00100.62	A	C
ATOM	1244	CG	ASP	A	221	16.920	114.778	21.101	1.00100.47	A	C
ATOM	1245	OD1	ASP	A	221	15.677	114.638	21.143	1.00100.93	A	O
ATOM	1246	OD2	ASP	A	221	17.683	113.933	20.591	1.00100.24	A	O
ATOM	1247	C	ASP	A	221	19.304	114.963	23.094	1.00 53.12	A	C
ATOM	1248	O	ASP	A	221	19.237	113.736	23.068	1.00 53.43	A	O
ATOM	1249	N	SER	A	222	20.459	115.620	23.103	1.00 50.42	A	N
ATOM	1250	CA	SER	A	222	21.744	114.932	23.034	1.00 51.84	A	C
ATOM	1251	CB	SER	A	222	22.811	115.896	22.499	1.00108.54	A	C
ATOM	1252	OG	SER	A	222	22.552	116.239	21.145	1.00107.30	A	O
ATOM	1253	C	SER	A	222	22.209	114.310	24.347	1.00 53.14	A	C
ATOM	1254	O	SER	A	222	22.544	113.122	24.399	1.00 53.64	A	O
ATOM	1255	N	MET	A	223	22.243	115.125	25.398	1.00 93.88	A	N
ATOM	1256	CA	MET	A	223	22.652	114.664	26.723	1.00 94.11	A	C
ATOM	1257	CB	MET	A	223	23.359	115.774	27.497	1.00 65.44	A	C
ATOM	1258	CG	MET	A	223	23.589	117.041	26.711	1.00 64.05	A	C
ATOM	1259	SD	MET	A	223	24.173	118.384	27.762	1.00 63.71	A	S
ATOM	1260	CE	MET	A	223	22.611	119.067	28.373	1.00 63.10	A	C
ATOM	1261	C	MET	A	223	21.412	114.252	27.505	1.00 94.32	A	C
ATOM	1262	O	MET	A	223	21.380	114.351	28.732	1.00 97.29	A	O
ATOM	1263	N	ALA	A	224	20.402	113.803	26.776	1.00115.21	A	N
ATOM	1264	CA	ALA	A	224	19.141	113.369	27.370	1.00115.42	A	C
ATOM	1265	CB	ALA	A	224	18.327	112.597	26.338	1.00104.19	A	C
ATOM	1266	C	ALA	A	224	19.272	112.538	28.638	1.00115.12	A	C
ATOM	1267	O	ALA	A	224	20.368	112.167	29.078	1.00114.85	A	O
ATOM	1268	N	ASN	A	225	18.106	112.239	29.206	1.00 80.78	A	N
ATOM	1269	CA	ASN	A	225	17.964	111.477	30.426	1.00 80.93	A	C
ATOM	1270	CB	ASN	A	225	17.329	110.118	30.111	1.00203.67	A	C
ATOM	1271	CG	ASN	A	225	15.823	110.177	30.212	1.00203.67	A	C
ATOM	1272	OD1	ASN	A	225	15.293	110.479	31.291	1.00203.67	A	O
ATOM	1273	ND2	ASN	A	225	15.097	109.948	29.107	1.00203.67	A	N
ATOM	1274	C	ASN	A	225	19.184	111.398	31.358	1.00 81.62	A	C
ATOM	1275	O	ASN	A	225	19.528	112.448	31.885	1.00 81.87	A	O
ATOM	1276	N	SER	A	226	19.835	110.247	31.537	1.00183.29	A	N
ATOM	1277	CA	SER	A	226	20.988	110.165	32.475	1.00183.13	A	C
ATOM	1278	CB	SER	A	226	22.369	110.232	31.766	1.00166.71	A	C
ATOM	1279	OG	SER	A	226	22.835	108.959	31.313	1.00166.57	A	O
ATOM	1280	C	SER	A	226	20.745	111.394	33.328	1.00182.94	A	C
ATOM	1281	O	SER	A	226	21.572	112.307	33.410	1.00183.02	A	O
ATOM	1282	N	PHE	A	227	19.553	111.405	33.927	1.00203.67	A	N
ATOM	1283	CA	PHE	A	227	19.053	112.557	34.669	1.00203.67	A	C
ATOM	1284	CB	PHE	A	227	17.518	112.572	34.604	1.00203.67	A	C

ATOM	1285	CG	PHE	A	227	16.935	113.853	34.066	1.00203.67	A	C
ATOM	1286	CD1	PHE	A	227	17.028	115.038	34.790	1.00203.67	A	C
ATOM	1287	CD2	PHE	A	227	16.306	113.869	32.829	1.00203.67	A	C
ATOM	1288	CE1	PHE	A	227	16.492	116.210	34.290	1.00203.67	A	C
ATOM	1289	CE2	PHE	A	227	15.768	115.031	32.325	1.00203.67	A	C
ATOM	1290	CZ	PHE	A	227	15.856	116.203	33.057	1.00203.67	A	C
ATOM	1291	C	PHE	A	227	19.471	112.904	36.086	1.00203.67	A	C
ATOM	1292	O	PHE	A	227	20.656	112.936	36.410	1.00203.67	A	O
ATOM	1293	N	VAL	A	228	18.470	113.210	36.899	1.00202.30	A	N
ATOM	1294	CA	VAL	A	228	18.675	113.609	38.286	1.00202.30	A	C
ATOM	1295	CB	VAL	A	228	17.325	113.762	39.020	1.00126.18	A	C
ATOM	1296	CG1	VAL	A	228	16.448	112.552	38.753	1.00126.47	A	C
ATOM	1297	CG2	VAL	A	228	17.563	113.909	40.513	1.00126.11	A	C
ATOM	1298	C	VAL	A	228	19.586	112.699	39.105	1.00202.30	A	C
ATOM	1299	O	VAL	A	228	20.780	112.964	39.222	1.00202.30	A	O
ATOM	1300	N	GLY	A	229	19.036	111.627	39.661	1.00121.71	A	N
ATOM	1301	CA	GLY	A	229	19.850	110.749	40.481	1.00119.74	A	C
ATOM	1302	C	GLY	A	229	19.973	111.385	41.854	1.00118.64	A	C
ATOM	1303	O	GLY	A	229	20.759	112.310	42.041	1.00118.26	A	O
ATOM	1304	N	THR	A	230	19.178	110.890	42.796	1.00114.88	A	N
ATOM	1305	CA	THR	A	230	19.125	111.362	44.186	1.00113.66	A	C
ATOM	1306	CB	THR	A	230	20.471	111.991	44.661	1.00 99.30	A	C
ATOM	1307	OG1	THR	A	230	21.495	110.990	44.632	1.00101.04	A	O
ATOM	1308	CG2	THR	A	230	20.355	112.514	46.095	1.00 98.89	A	C
ATOM	1309	C	THR	A	230	17.985	112.361	44.388	1.00111.81	A	C
ATOM	1310	O	THR	A	230	16.835	111.952	44.559	1.00110.80	A	O
ATOM	1311	N	ARG	A	231	18.297	113.653	44.357	1.00 50.63	A	N
ATOM	1312	CA	ARG	A	231	17.306	114.708	44.555	1.00 47.01	A	C
ATOM	1313	CB	ARG	A	231	17.939	115.843	45.341	1.00 73.50	A	C
ATOM	1314	CG	ARG	A	231	18.659	115.425	46.600	1.00 76.79	A	C
ATOM	1315	CD	ARG	A	231	19.589	116.556	47.031	1.00 80.20	A	C
ATOM	1316	NE	ARG	A	231	19.173	117.863	46.498	1.00 83.47	A	N
ATOM	1317	CZ	ARG	A	231	19.784	119.018	46.755	1.00 84.03	A	C
ATOM	1318	NH1	ARG	A	231	20.848	119.052	47.550	1.00 84.51	A	N
ATOM	1319	NH2	ARG	A	231	19.356	120.146	46.202	1.00 83.92	A	N
ATOM	1320	C	ARG	A	231	16.795	115.267	43.233	1.00 44.29	A	C
ATOM	1321	O	ARG	A	231	17.551	115.871	42.488	1.00 44.44	A	O
ATOM	1322	N	SER	A	232	15.511	115.079	42.945	1.00 37.83	A	N
ATOM	1323	CA	SER	A	232	14.929	115.596	41.709	1.00 33.87	A	C
ATOM	1324	CB	SER	A	232	13.983	114.564	41.086	1.00 41.67	A	C
ATOM	1325	OG	SER	A	232	12.955	114.193	41.991	1.00 40.66	A	O
ATOM	1326	C	SER	A	232	14.170	116.892	41.979	1.00 30.67	A	C
ATOM	1327	O	SER	A	232	13.808	117.202	43.112	1.00 30.75	A	O

ATOM	1328	N	TYR A 233	13.959	117.664	40.915	1.00	47.41	A	N
ATOM	1329	CA	TYR A 233	13.225	118.912	41.007	1.00	43.54	A	C
ATOM	1330	CB	TYR A 233	14.156	120.105	40.755	1.00	22.72	A	C
ATOM	1331	CG	TYR A 233	15.012	120.501	41.941	1.00	17.80	A	C
ATOM	1332	CD1	TYR A 233	14.474	121.217	42.999	1.00	17.68	A	C
ATOM	1333	CE1	TYR A 233	15.259	121.598	44.074	1.00	17.07	A	C
ATOM	1334	CD2	TYR A 233	16.366	120.172	41.997	1.00	15.44	A	C
ATOM	1335	CE2	TYR A 233	17.162	120.550	43.072	1.00	15.13	A	C
ATOM	1336	CZ	TYR A 233	16.597	121.264	44.103	1.00	15.74	A	C
ATOM	1337	OH	TYR A 233	17.337	121.666	45.176	1.00	14.60	A	O
ATOM	1338	C	TYR A 233	12.119	118.866	39.956	1.00	44.02	A	C
ATOM	1339	O	TYR A 233	11.456	119.867	39.682	1.00	45.41	A	O
ATOM	1340	N	MET A 234	11.924	117.687	39.379	1.00	39.23	A	N
ATOM	1341	CA	MET A 234	10.919	117.490	38.352	1.00	37.91	A	C
ATOM	1342	CB	MET A 234	11.179	116.206	37.596	1.00	60.51	A	C
ATOM	1343	CG	MET A 234	12.009	116.384	36.363	1.00	62.85	A	C
ATOM	1344	SD	MET A 234	12.429	114.770	35.676	1.00	65.21	A	S
ATOM	1345	CE	MET A 234	14.198	114.506	36.245	1.00	64.29	A	C
ATOM	1346	C	MET A 234	9.559	117.411	38.958	1.00	36.94	A	C
ATOM	1347	O	MET A 234	9.363	116.699	39.933	1.00	36.32	A	O
ATOM	1348	N	ALA A 235	8.618	118.134	38.368	1.00	24.72	A	N
ATOM	1349	CA	ALA A 235	7.252	118.152	38.850	1.00	25.89	A	C
ATOM	1350	CB	ALA A 235	6.443	119.143	38.049	1.00	51.94	A	C
ATOM	1351	C	ALA A 235	6.674	116.768	38.688	1.00	26.75	A	C
ATOM	1352	O	ALA A 235	7.068	116.023	37.797	1.00	27.54	A	O
ATOM	1353	N	PRO A 236	5.729	116.401	39.561	1.00	26.89	A	N
ATOM	1354	CD	PRO A 236	5.094	117.297	40.536	1.00	12.25	A	C
ATOM	1355	CA	PRO A 236	5.061	115.099	39.544	1.00	27.95	A	C
ATOM	1356	CB	PRO A 236	3.782	115.368	40.325	1.00	11.39	A	C
ATOM	1357	CG	PRO A 236	4.223	116.347	41.332	1.00	12.09	A	C
ATOM	1358	C	PRO A 236	4.763	114.696	38.106	1.00	29.59	A	C
ATOM	1359	O	PRO A 236	4.984	113.561	37.708	1.00	30.04	A	O
ATOM	1360	N	GLU A 237	4.264	115.679	37.364	1.00	23.55	A	N
ATOM	1361	CA	GLU A 237	3.874	115.578	35.958	1.00	24.81	A	C
ATOM	1362	CB	GLU A 237	3.318	116.926	35.503	1.00	41.40	A	C
ATOM	1363	CG	GLU A 237	3.639	118.042	36.456	1.00	40.26	A	C
ATOM	1364	CD	GLU A 237	3.898	119.316	35.731	1.00	39.49	A	C
ATOM	1365	OE1	GLU A 237	4.157	120.341	36.399	1.00	39.40	A	O
ATOM	1366	OE2	GLU A 237	3.844	119.285	34.483	1.00	37.88	A	O
ATOM	1367	C	GLU A 237	4.965	115.130	34.974	1.00	26.07	A	C
ATOM	1368	O	GLU A 237	4.741	114.131	34.295	1.00	27.52	A	O
ATOM	1369	N	ARG A 238	6.072	115.799	34.879	1.00	74.49	A	N
ATOM	1370	CA	ARG A 238	7.065	115.312	33.921	1.00	77.86	A	C

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ATOM   1371  CB  ARG A 238      8.036 116.394  33.452  1.00119.18      A    C
ATOM   1372  CG  ARG A 238      8.760 115.896  32.214  1.00124.27      A    C
ATOM   1373  CD  ARG A 238      9.818 116.799  31.620  1.00129.12      A    C
ATOM   1374  NE  ARG A 238     10.405 116.111  30.467  1.00134.45      A    N
ATOM   1375  CZ  ARG A 238     11.386 116.581  29.702  1.00136.53      A    C
ATOM   1376  NH1 ARG A 238     11.835 115.859  28.682  1.00137.34      A    N
ATOM   1377  NH2 ARG A 238     11.921 117.768  29.948  1.00138.23      A    N
ATOM   1378  C   ARG A 238      7.838 114.127  34.455  1.00 78.98      A    C
ATOM   1379  O   ARG A 238      8.959 113.846  34.042  1.00 79.41      A    O
ATOM   1380  N   LEU A 239      7.223 113.442  35.419  1.00 43.85      A    N
ATOM   1381  CA  LEU A 239      7.797 112.244  35.995  1.00 44.89      A    C
ATOM   1382  CB  LEU A 239      7.846 112.302  37.526  1.00 12.83      A    C
ATOM   1383  CG  LEU A 239      8.962 113.115  38.212  1.00 10.51      A    C
ATOM   1384  CD1 LEU A 239      8.931 112.764  39.683  1.00  6.96      A    C
ATOM   1385  CD2 LEU A 239     10.369 112.831  37.640  1.00  8.81      A    C
ATOM   1386  C   LEU A 239      6.773 111.231  35.548  1.00 47.18      A    C
ATOM   1387  O   LEU A 239      7.086 110.297  34.809  1.00 46.02      A    O
ATOM   1388  N   GLN A 240      5.537 111.447  35.982  1.00 41.08      A    N
ATOM   1389  CA  GLN A 240      4.442 110.588  35.596  1.00 45.44      A    C
ATOM   1390  CB  GLN A 240      3.172 110.960  36.353  1.00186.67      A    C
ATOM   1391  CG  GLN A 240      2.015 110.044  36.050  1.00187.75      A    C
ATOM   1392  CD  GLN A 240      0.737 110.506  36.701  1.00189.86      A    C
ATOM   1393  OE1 GLN A 240     -0.320 109.887  36.535  1.00192.76      A    O
ATOM   1394  NE2 GLN A 240      0.820 111.602  37.451  1.00190.51      A    N
ATOM   1395  C   GLN A 240      4.275 110.891  34.119  1.00 48.89      A    C
ATOM   1396  O   GLN A 240      3.382 111.630  33.730  1.00 49.42      A    O
ATOM   1397  N   GLY A 241      5.149 110.332  33.294  1.00 60.71      A    N
ATOM   1398  CA  GLY A 241      5.061 110.588  31.873  1.00 65.43      A    C
ATOM   1399  C   GLY A 241      6.101 111.620  31.519  1.00 69.18      A    C
ATOM   1400  O   GLY A 241      7.181 111.639  32.107  1.00 69.40      A    O
ATOM   1401  N   THR A 242      5.786 112.476  30.561  1.00 88.15      A    N
ATOM   1402  CA  THR A 242      6.712 113.516  30.151  1.00 89.76      A    C
ATOM   1403  CB  THR A 242      7.881 112.932  29.321  1.00203.67      A    C
ATOM   1404  OG1 THR A 242      8.732 113.995  28.871  1.00203.67      A    O
ATOM   1405  CG2 THR A 242      7.360 112.157  28.119  1.00203.67      A    C
ATOM   1406  C   THR A 242      5.972 114.559  29.332  1.00 91.42      A    C
ATOM   1407  O   THR A 242      5.349 114.238  28.325  1.00 93.93      A    O
ATOM   1408  N   HIS A 243      6.022 115.808  29.790  1.00 45.09      A    N
ATOM   1409  CA  HIS A 243      5.361 116.921  29.110  1.00 45.17      A    C
ATOM   1410  CB  HIS A 243      3.855 116.817  29.282  1.00 70.28      A    C
ATOM   1411  CG  HIS A 243      3.440 115.704  30.185  1.00 71.67      A    C
ATOM   1412  CD2 HIS A 243      3.163 115.681  31.511  1.00 72.42      A    C
ATOM   1413  ND1 HIS A 243      3.322 114.406  29.745  1.00 72.24      A    N
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ATOM   1414  CE1 HIS A 243      2.987 113.628  30.759  1.00 73.16      A    C
ATOM   1415  NE2 HIS A 243      2.881 114.378  31.843  1.00 73.26      A    N
ATOM   1416  C   HIS A 243      5.840 118.232  29.732  1.00 44.54      A    C
ATOM   1417  O   HIS A 243      5.064 118.924  30.395  1.00 45.04      A    O
ATOM   1418  N   TYR A 244      7.102 118.564  29.518  1.00 76.08      A    N
ATOM   1419  CA  TYR A 244      7.651 119.788  30.081  1.00 74.49      A    C
ATOM   1420  CB  TYR A 244      9.108 119.956  29.693  1.00 67.10      A    C
ATOM   1421  CG  TYR A 244      9.849 120.725  30.739  1.00 70.19      A    C
ATOM   1422  CD1 TYR A 244     10.334 120.091  31.870  1.00 72.03      A    C
ATOM   1423  CE1 TYR A 244     10.938 120.798  32.876  1.00 73.61      A    C
ATOM   1424  CD2 TYR A 244      9.994 122.096  30.643  1.00 70.42      A    C
ATOM   1425  CE2 TYR A 244     10.595 122.816  31.646  1.00 72.12      A    C
ATOM   1426  CZ  TYR A 244     11.065 122.164  32.762  1.00 73.52      A    C
ATOM   1427  OH  TYR A 244     11.654 122.882  33.775  1.00 75.14      A    O
ATOM   1428  C   TYR A 244      6.893 121.017  29.632  1.00 70.59      A    C
ATOM   1429  O   TYR A 244      6.987 121.452  28.490  1.00 70.62      A    O
ATOM   1430  N   SER A 245      6.126 121.576  30.566  1.00 46.31      A    N
ATOM   1431  CA  SER A 245      5.348 122.768  30.306  1.00 41.50      A    C
ATOM   1432  CB  SER A 245      4.000 122.672  31.023  1.00 54.63      A    C
ATOM   1433  OG  SER A 245      3.206 123.816  30.786  1.00 56.06      A    O
ATOM   1434  C   SER A 245      6.142 123.920  30.877  1.00 38.46      A    C
ATOM   1435  O   SER A 245      7.364 123.885  30.937  1.00 40.39      A    O
ATOM   1436  N   VAL A 246      5.430 124.951  31.301  1.00 41.06      A    N
ATOM   1437  CA  VAL A 246      6.039 126.115  31.911  1.00 37.79      A    C
ATOM   1438  CB  VAL A 246      5.294 127.408  31.517  1.00 29.02      A    C
ATOM   1439  CG1 VAL A 246      6.154 128.613  31.809  1.00 27.27      A    C
ATOM   1440  CG2 VAL A 246      4.898 127.355  30.049  1.00 29.13      A    C
ATOM   1441  C   VAL A 246      5.767 125.829  33.366  1.00 34.07      A    C
ATOM   1442  O   VAL A 246      6.573 126.116  34.230  1.00 33.11      A    O
ATOM   1443  N   GLN A 247      4.604 125.229  33.595  1.00 35.73      A    N
ATOM   1444  CA  GLN A 247      4.110 124.857  34.911  1.00 30.75      A    C
ATOM   1445  CB  GLN A 247      2.822 124.055  34.772  1.00 63.51      A    C
ATOM   1446  CG  GLN A 247      1.916 124.520  33.668  1.00 66.34      A    C
ATOM   1447  CD  GLN A 247      1.507 125.944  33.852  1.00 68.42      A    C
ATOM   1448  OE1 GLN A 247      1.308 126.394  34.979  1.00 70.92      A    O
ATOM   1449  NE2 GLN A 247      1.361 126.672  32.746  1.00 69.35      A    N
ATOM   1450  C   GLN A 247      5.117 124.004  35.660  1.00 29.18      A    C
ATOM   1451  O   GLN A 247      5.038 123.845  36.884  1.00 29.36      A    O
ATOM   1452  N   SER A 248      6.053 123.427  34.925  1.00 29.95      A    N
ATOM   1453  CA  SER A 248      7.049 122.597  35.562  1.00 28.20      A    C
ATOM   1454  CB  SER A 248      7.580 121.593  34.553  1.00 10.01      A    C
ATOM   1455  OG  SER A 248      6.520 120.766  34.098  1.00  9.31      A    O
ATOM   1456  C   SER A 248      8.155 123.468  36.164  1.00 26.29      A    C
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ATOM	1457	O	SER	A	248	8.574	123.230	37.287	1.00	26.36	A	O
ATOM	1458	N	ASP	A	249	8.607	124.487	35.435	1.00	21.00	A	N
ATOM	1459	CA	ASP	A	249	9.628	125.394	35.955	1.00	19.49	A	C
ATOM	1460	CB	ASP	A	249	9.947	126.505	34.969	1.00	26.12	A	C
ATOM	1461	CG	ASP	A	249	10.677	126.004	33.769	1.00	27.48	A	C
ATOM	1462	OD1	ASP	A	249	11.648	125.260	33.960	1.00	28.22	A	O
ATOM	1463	OD2	ASP	A	249	10.295	126.347	32.631	1.00	28.78	A	O
ATOM	1464	C	ASP	A	249	9.073	126.024	37.201	1.00	18.46	A	C
ATOM	1465	O	ASP	A	249	9.751	126.119	38.226	1.00	19.31	A	O
ATOM	1466	N	ILE	A	250	7.832	126.477	37.091	1.00	16.36	A	N
ATOM	1467	CA	ILE	A	250	7.163	127.086	38.211	1.00	13.55	A	C
ATOM	1468	CB	ILE	A	250	5.673	127.311	37.941	1.00	20.29	A	C
ATOM	1469	CG2	ILE	A	250	4.939	127.408	39.235	1.00	20.41	A	C
ATOM	1470	CG1	ILE	A	250	5.450	128.612	37.173	1.00	20.29	A	C
ATOM	1471	CD1	ILE	A	250	5.960	128.580	35.788	1.00	20.29	A	C
ATOM	1472	C	ILE	A	250	7.312	126.132	39.374	1.00	14.03	A	C
ATOM	1473	O	ILE	A	250	7.626	126.566	40.473	1.00	14.18	A	O
ATOM	1474	N	TRP	A	251	7.104	124.832	39.136	1.00	22.50	A	N
ATOM	1475	CA	TRP	A	251	7.235	123.829	40.202	1.00	22.48	A	C
ATOM	1476	CB	TRP	A	251	6.835	122.434	39.710	1.00	23.28	A	C
ATOM	1477	CG	TRP	A	251	7.258	121.318	40.650	1.00	23.28	A	C
ATOM	1478	CD2	TRP	A	251	6.429	120.593	41.567	1.00	23.28	A	C
ATOM	1479	CE2	TRP	A	251	7.264	119.703	42.271	1.00	23.68	A	C
ATOM	1480	CE3	TRP	A	251	5.064	120.612	41.862	1.00	23.28	A	C
ATOM	1481	CD1	TRP	A	251	8.523	120.840	40.832	1.00	23.28	A	C
ATOM	1482	NE1	TRP	A	251	8.536	119.872	41.802	1.00	23.28	A	N
ATOM	1483	CZ2	TRP	A	251	6.783	118.845	43.249	1.00	23.84	A	C
ATOM	1484	CZ3	TRP	A	251	4.582	119.760	42.832	1.00	23.64	A	C
ATOM	1485	CH2	TRP	A	251	5.440	118.888	43.518	1.00	24.78	A	C
ATOM	1486	C	TRP	A	251	8.654	123.777	40.741	1.00	22.48	A	C
ATOM	1487	O	TRP	A	251	8.872	123.841	41.939	1.00	22.52	A	O
ATOM	1488	N	SER	A	252	9.623	123.652	39.851	1.00	18.78	A	N
ATOM	1489	CA	SER	A	252	11.011	123.605	40.263	1.00	20.04	A	C
ATOM	1490	CB	SER	A	252	11.909	123.428	39.039	1.00	29.86	A	C
ATOM	1491	OG	SER	A	252	11.671	122.176	38.418	1.00	34.06	A	O
ATOM	1492	C	SER	A	252	11.395	124.867	41.039	1.00	19.68	A	C
ATOM	1493	O	SER	A	252	12.300	124.829	41.870	1.00	21.46	A	O
ATOM	1494	N	MET	A	253	10.716	125.985	40.778	1.00	15.76	A	N
ATOM	1495	CA	MET	A	253	11.013	127.211	41.514	1.00	16.96	A	C
ATOM	1496	CB	MET	A	253	10.404	128.431	40.836	1.00	21.07	A	C
ATOM	1497	CG	MET	A	253	10.728	129.740	41.569	1.00	22.82	A	C
ATOM	1498	SD	MET	A	253	10.120	131.224	40.766	1.00	24.37	A	S
ATOM	1499	CE	MET	A	253	8.344	130.888	40.865	1.00	24.40	A	C

ATOM	1500	C	MET	A	253	10.476	127.122	42.937	1.00	16.57	A	C
ATOM	1501	O	MET	A	253	11.172	127.468	43.895	1.00	17.32	A	O
ATOM	1502	N	GLY	A	254	9.235	126.653	43.063	1.00	24.19	A	N
ATOM	1503	CA	GLY	A	254	8.595	126.499	44.365	1.00	23.51	A	C
ATOM	1504	C	GLY	A	254	9.368	125.574	45.281	1.00	23.51	A	C
ATOM	1505	O	GLY	A	254	9.570	125.860	46.461	1.00	23.57	A	O
ATOM	1506	N	LEU	A	255	9.800	124.447	44.736	1.00	30.88	A	N
ATOM	1507	CA	LEU	A	255	10.580	123.520	45.518	1.00	30.88	A	C
ATOM	1508	CB	LEU	A	255	10.812	122.228	44.747	1.00	27.13	A	C
ATOM	1509	CG	LEU	A	255	11.235	121.111	45.695	1.00	26.31	A	C
ATOM	1510	CD1	LEU	A	255	9.990	120.562	46.374	1.00	26.57	A	C
ATOM	1511	CD2	LEU	A	255	11.974	120.027	44.949	1.00	26.68	A	C
ATOM	1512	C	LEU	A	255	11.931	124.173	45.837	1.00	33.11	A	C
ATOM	1513	O	LEU	A	255	12.474	123.996	46.925	1.00	30.88	A	O
ATOM	1514	N	SER	A	256	12.469	124.933	44.887	1.00	42.19	A	N
ATOM	1515	CA	SER	A	256	13.752	125.597	45.082	1.00	41.87	A	C
ATOM	1516	CB	SER	A	256	14.243	126.191	43.768	1.00	26.18	A	C
ATOM	1517	OG	SER	A	256	14.631	125.171	42.874	1.00	27.27	A	O
ATOM	1518	C	SER	A	256	13.702	126.688	46.144	1.00	42.01	A	C
ATOM	1519	O	SER	A	256	14.694	126.933	46.838	1.00	41.23	A	O
ATOM	1520	N	LEU	A	257	12.556	127.350	46.261	1.00	31.99	A	N
ATOM	1521	CA	LEU	A	257	12.394	128.396	47.262	1.00	32.06	A	C
ATOM	1522	CB	LEU	A	257	11.124	129.219	46.976	1.00	22.21	A	C
ATOM	1523	CG	LEU	A	257	11.205	130.588	46.290	1.00	21.67	A	C
ATOM	1524	CD1	LEU	A	257	12.493	130.734	45.513	1.00	21.14	A	C
ATOM	1525	CD2	LEU	A	257	10.000	130.750	45.379	1.00	23.42	A	C
ATOM	1526	C	LEU	A	257	12.307	127.747	48.648	1.00	34.23	A	C
ATOM	1527	O	LEU	A	257	12.984	128.174	49.590	1.00	35.10	A	O
ATOM	1528	N	VAL	A	258	11.475	126.713	48.765	1.00	24.04	A	N
ATOM	1529	CA	VAL	A	258	11.319	126.005	50.025	1.00	24.21	A	C
ATOM	1530	CB	VAL	A	258	10.330	124.859	49.892	1.00	11.72	A	C
ATOM	1531	CG1	VAL	A	258	10.487	123.908	51.066	1.00	12.01	A	C
ATOM	1532	CG2	VAL	A	258	8.927	125.398	49.860	1.00	10.67	A	C
ATOM	1533	C	VAL	A	258	12.643	125.429	50.525	1.00	25.33	A	C
ATOM	1534	O	VAL	A	258	12.850	125.265	51.727	1.00	25.66	A	O
ATOM	1535	N	GLU	A	259	13.534	125.113	49.592	1.00	23.91	A	N
ATOM	1536	CA	GLU	A	259	14.839	124.566	49.929	1.00	22.93	A	C
ATOM	1537	CB	GLU	A	259	15.539	124.073	48.667	1.00	46.78	A	C
ATOM	1538	CG	GLU	A	259	16.939	123.540	48.904	1.00	47.15	A	C
ATOM	1539	CD	GLU	A	259	17.351	122.502	47.874	1.00	45.54	A	C
ATOM	1540	OE1	GLU	A	259	18.564	122.256	47.726	1.00	44.00	A	O
ATOM	1541	OE2	GLU	A	259	16.461	121.922	47.220	1.00	44.40	A	O
ATOM	1542	C	GLU	A	259	15.678	125.627	50.607	1.00	23.21	A	C

ATOM	1543	O	GLU	A	259	16.098	125.458	51.743	1.00	21.22	A	O
ATOM	1544	N	LEU	A	260	15.905	126.727	49.900	1.00	29.08	A	N
ATOM	1545	CA	LEU	A	260	16.688	127.854	50.406	1.00	29.17	A	C
ATOM	1546	CB	LEU	A	260	16.825	128.907	49.318	1.00	8.66	A	C
ATOM	1547	CG	LEU	A	260	17.583	128.457	48.080	1.00	10.10	A	C
ATOM	1548	CD1	LEU	A	260	17.187	129.323	46.889	1.00	9.89	A	C
ATOM	1549	CD2	LEU	A	260	19.086	128.516	48.380	1.00	9.05	A	C
ATOM	1550	C	LEU	A	260	16.027	128.481	51.621	1.00	28.89	A	C
ATOM	1551	O	LEU	A	260	16.672	129.174	52.406	1.00	27.14	A	O
ATOM	1552	N	ALA	A	261	14.731	128.234	51.762	1.00	44.26	A	N
ATOM	1553	CA	ALA	A	261	13.977	128.769	52.880	1.00	44.28	A	C
ATOM	1554	CB	ALA	A	261	12.499	128.828	52.520	1.00	102.24	A	C
ATOM	1555	C	ALA	A	261	14.178	127.940	54.150	1.00	43.25	A	C
ATOM	1556	O	ALA	A	261	14.289	128.475	55.251	1.00	44.09	A	O
ATOM	1557	N	VAL	A	262	14.245	126.631	53.995	1.00	13.81	A	N
ATOM	1558	CA	VAL	A	262	14.403	125.764	55.137	1.00	13.99	A	C
ATOM	1559	CB	VAL	A	262	13.421	124.604	55.025	1.00	11.33	A	C
ATOM	1560	CG1	VAL	A	262	13.723	123.561	56.060	1.00	11.22	A	C
ATOM	1561	CG2	VAL	A	262	12.012	125.129	55.194	1.00	11.14	A	C
ATOM	1562	C	VAL	A	262	15.821	125.241	55.350	1.00	15.56	A	C
ATOM	1563	O	VAL	A	262	16.168	124.797	56.444	1.00	13.43	A	O
ATOM	1564	N	GLY	A	263	16.656	125.281	54.324	1.00	30.40	A	N
ATOM	1565	CA	GLY	A	263	18.014	124.810	54.525	1.00	31.79	A	C
ATOM	1566	C	GLY	A	263	18.345	123.431	53.987	1.00	32.88	A	C
ATOM	1567	O	GLY	A	263	19.509	123.025	53.977	1.00	34.12	A	O
ATOM	1568	N	ARG	A	264	17.339	122.696	53.539	1.00	22.31	A	N
ATOM	1569	CA	ARG	A	264	17.613	121.388	52.987	1.00	23.20	A	C
ATOM	1570	CB	ARG	A	264	17.514	120.318	54.069	1.00	77.11	A	C
ATOM	1571	CG	ARG	A	264	16.110	119.885	54.360	1.00	82.08	A	C
ATOM	1572	CD	ARG	A	264	16.084	118.927	55.510	1.00	85.94	A	C
ATOM	1573	NE	ARG	A	264	15.186	117.817	55.250	1.00	89.65	A	N
ATOM	1574	CZ	ARG	A	264	14.770	116.982	56.189	1.00	92.90	A	C
ATOM	1575	NH1	ARG	A	264	13.953	115.985	55.872	1.00	94.99	A	N
ATOM	1576	NH2	ARG	A	264	15.164	117.156	57.450	1.00	94.91	A	N
ATOM	1577	C	ARG	A	264	16.644	121.062	51.878	1.00	23.61	A	C
ATOM	1578	O	ARG	A	264	15.633	121.738	51.700	1.00	22.37	A	O
ATOM	1579	N	TYR	A	265	16.982	120.026	51.118	1.00	25.52	A	N
ATOM	1580	CA	TYR	A	265	16.129	119.584	50.042	1.00	25.01	A	C
ATOM	1581	CB	TYR	A	265	16.789	118.447	49.270	1.00	12.79	A	C
ATOM	1582	CG	TYR	A	265	15.917	117.839	48.195	1.00	11.37	A	C
ATOM	1583	CD1	TYR	A	265	15.550	118.546	47.060	1.00	11.20	A	C
ATOM	1584	CE1	TYR	A	265	14.792	117.935	46.055	1.00	11.51	A	C
ATOM	1585	CD2	TYR	A	265	15.500	116.530	48.294	1.00	10.81	A	C

ATOM	1586	CE2	TYR A 265	14.762	115.928	47.307	1.00	10.23	A	C
ATOM	1587	CZ	TYR A 265	14.411	116.619	46.196	1.00	10.15	A	C
ATOM	1588	OH	TYR A 265	13.700	115.972	45.222	1.00	8.54	A	O
ATOM	1589	C	TYR A 265	14.900	119.108	50.778	1.00	28.16	A	C
ATOM	1590	O	TYR A 265	14.925	118.134	51.514	1.00	28.48	A	O
ATOM	1591	N	PRO A 266	13.801	119.824	50.607	1.00	20.07	A	N
ATOM	1592	CD	PRO A 266	13.620	120.977	49.718	1.00	36.60	A	C
ATOM	1593	CA	PRO A 266	12.553	119.467	51.277	1.00	21.90	A	C
ATOM	1594	CB	PRO A 266	11.588	120.542	50.801	1.00	39.09	A	C
ATOM	1595	CG	PRO A 266	12.151	120.953	49.466	1.00	37.63	A	C
ATOM	1596	C	PRO A 266	12.010	118.066	51.066	1.00	27.55	A	C
ATOM	1597	O	PRO A 266	11.962	117.281	52.004	1.00	29.14	A	O
ATOM	1598	N	ILE A 267	11.610	117.763	49.822	1.00	118.97	A	N
ATOM	1599	CA	ILE A 267	11.011	116.473	49.458	1.00	120.11	A	C
ATOM	1600	CB	ILE A 267	11.624	115.830	48.249	1.00	60.15	A	C
ATOM	1601	CG2	ILE A 267	11.242	114.313	48.215	1.00	59.04	A	C
ATOM	1602	CG1	ILE A 267	11.079	116.524	47.017	1.00	59.01	A	C
ATOM	1603	CD1	ILE A 267	9.652	116.879	47.204	1.00	58.07	A	C
ATOM	1604	C	ILE A 267	10.936	115.390	50.466	1.00	125.16	A	C
ATOM	1605	O	ILE A 267	9.874	114.837	50.699	1.00	125.24	A	O
ATOM	1606	N	PRO A 268	12.068	114.962	51.025	1.00	53.93	A	N
ATOM	1607	CD	PRO A 268	13.495	115.014	50.670	1.00	35.94	A	C
ATOM	1608	CA	PRO A 268	11.801	113.907	52.002	1.00	53.27	A	C
ATOM	1609	CB	PRO A 268	13.146	113.204	52.113	1.00	39.49	A	C
ATOM	1610	CG	PRO A 268	14.106	114.335	51.867	1.00	37.41	A	C
ATOM	1611	C	PRO A 268	11.396	114.579	53.323	1.00	58.09	A	C
ATOM	1612	O	PRO A 268	12.238	115.082	54.036	1.00	57.93	A	O
ATOM	1613	N	PRO A 269	10.082	114.608	53.649	1.00	120.81	A	N
ATOM	1614	CD	PRO A 269	9.166	113.574	53.144	1.00	203.67	A	C
ATOM	1615	CA	PRO A 269	9.545	115.210	54.874	1.00	119.67	A	C
ATOM	1616	CB	PRO A 269	8.683	114.098	55.424	1.00	203.67	A	C
ATOM	1617	CG	PRO A 269	8.011	113.636	54.150	1.00	203.67	A	C
ATOM	1618	C	PRO A 269	10.639	115.680	55.837	1.00	122.77	A	C
ATOM	1619	O	PRO A 269	11.445	114.882	56.311	1.00	123.52	A	O
ATOM	1620	N	PRO A 270	10.669	116.978	56.147	1.00	130.19	A	N
ATOM	1621	CD	PRO A 270	9.609	117.951	55.890	1.00	51.48	A	C
ATOM	1622	CA	PRO A 270	11.676	117.549	57.041	1.00	127.82	A	C
ATOM	1623	CB	PRO A 270	11.368	119.052	57.016	1.00	52.87	A	C
ATOM	1624	CG	PRO A 270	10.414	119.217	55.887	1.00	52.68	A	C
ATOM	1625	C	PRO A 270	11.632	116.999	58.448	1.00	128.46	A	C
ATOM	1626	O	PRO A 270	12.358	116.051	58.777	1.00	126.60	A	O
ATOM	1627	N	ASP A 271	10.772	117.591	59.276	1.00	192.23	A	N
ATOM	1628	CA	ASP A 271	10.645	117.195	60.669	1.00	191.08	A	C

ATOM	1629	CB	ASP	A	271	10.242	115.717	60.750	1.00 75.02	A	C
ATOM	1630	CG	ASP	A	271	10.484	115.120	62.113	1.00 75.77	A	C
ATOM	1631	OD1	ASP	A	271	11.663	114.907	62.470	1.00 75.51	A	O
ATOM	1632	OD2	ASP	A	271	9.492	114.867	62.825	1.00 76.42	A	O
ATOM	1633	C	ASP	A	271	12.003	117.474	61.342	1.00191.86	A	C
ATOM	1634	O	ASP	A	271	12.902	116.622	61.343	1.00191.44	A	O
ATOM	1635	N	ALA	A	272	12.131	118.686	61.891	1.00 98.30	A	N
ATOM	1636	CA	ALA	A	272	13.364	119.145	62.544	1.00 98.14	A	C
ATOM	1637	CB	ALA	A	272	14.532	118.814	61.673	1.00 15.10	A	C
ATOM	1638	C	ALA	A	272	13.390	120.652	62.844	1.00 99.21	A	C
ATOM	1639	O	ALA	A	272	12.348	121.298	62.937	1.00 99.39	A	O
ATOM	1640	N	LYS	A	273	14.606	121.188	62.977	1.00 65.32	A	N
ATOM	1641	CA	LYS	A	273	14.846	122.617	63.250	1.00 66.46	A	C
ATOM	1642	CB	LYS	A	273	15.721	122.791	64.508	1.00 4.67	A	C
ATOM	1643	CG	LYS	A	273	14.956	122.630	65.798	1.00 4.67	A	C
ATOM	1644	CD	LYS	A	273	13.800	123.627	65.941	1.00 4.67	A	C
ATOM	1645	CE	LYS	A	273	12.476	123.116	65.355	1.00 5.66	A	C
ATOM	1646	NZ	LYS	A	273	12.251	123.438	63.894	1.00 6.41	A	N
ATOM	1647	C	LYS	A	273	15.488	123.377	62.075	1.00 66.44	A	C
ATOM	1648	O	LYS	A	273	15.839	124.560	62.194	1.00 65.91	A	O
ATOM	1649	N	ASP	A	311	19.688	112.154	63.895	1.00178.38	A	N
ATOM	1650	CA	ASP	A	311	20.423	112.413	65.128	1.00179.40	A	C
ATOM	1651	CB	ASP	A	311	19.938	113.723	65.761	1.00158.88	A	C
ATOM	1652	CG	ASP	A	311	20.664	114.055	67.052	1.00158.62	A	C
ATOM	1653	OD1	ASP	A	311	20.436	115.158	67.593	1.00157.70	A	O
ATOM	1654	OD2	ASP	A	311	21.459	113.216	67.529	1.00158.55	A	O
ATOM	1655	C	ASP	A	311	20.245	111.260	66.111	1.00179.42	A	C
ATOM	1656	O	ASP	A	311	19.816	110.170	65.732	1.00179.43	A	O
ATOM	1657	N	SER	A	312	22.642	110.131	60.919	1.00190.27	A	N
ATOM	1658	CA	SER	A	312	21.367	110.833	60.835	1.00188.90	A	C
ATOM	1659	CB	SER	A	312	21.604	112.323	60.565	1.00160.42	A	C
ATOM	1660	OG	SER	A	312	22.470	112.898	61.532	1.00160.30	A	O
ATOM	1661	C	SER	A	312	20.522	110.233	59.713	1.00187.76	A	C
ATOM	1662	O	SER	A	312	21.038	109.493	58.873	1.00186.93	A	O
ATOM	1663	N	ARG	A	313	19.228	110.548	59.703	1.00203.67	A	N
ATOM	1664	CA	ARG	A	313	18.334	110.034	58.670	1.00203.67	A	C
ATOM	1665	CB	ARG	A	313	16.958	110.709	58.738	1.00 98.77	A	C
ATOM	1666	CG	ARG	A	313	16.001	110.125	59.764	1.00 99.54	A	C
ATOM	1667	CD	ARG	A	313	14.557	110.341	59.326	1.00 99.90	A	C
ATOM	1668	NE	ARG	A	313	14.242	109.588	58.110	1.00101.08	A	N
ATOM	1669	CZ	ARG	A	313	13.097	109.683	57.438	1.00101.58	A	C
ATOM	1670	NH1	ARG	A	313	12.144	110.507	57.859	1.00100.91	A	N
ATOM	1671	NH2	ARG	A	313	12.899	108.950	56.349	1.00101.49	A	N

ATOM	1672	C	ARG	A	313	18.928	110.257	57.286	1.00203.67	A	C
ATOM	1673	O	ARG	A	313	19.038	111.391	56.815	1.00203.67	A	O
ATOM	1674	N	PRO	A	314	19.326	109.167	56.620	1.00167.83	A	N
ATOM	1675	CD	PRO	A	314	19.371	107.811	57.193	1.00195.98	A	C
ATOM	1676	CA	PRO	A	314	19.920	109.189	55.279	1.00164.36	A	C
ATOM	1677	CB	PRO	A	314	20.262	107.719	55.033	1.00194.24	A	C
ATOM	1678	CG	PRO	A	314	20.501	107.187	56.422	1.00195.13	A	C
ATOM	1679	C	PRO	A	314	18.980	109.746	54.209	1.00160.39	A	C
ATOM	1680	O	PRO	A	314	17.898	110.254	54.508	1.00159.44	A	O
ATOM	1681	N	ALA	A	315	19.408	109.648	52.958	1.00104.00	A	N
ATOM	1682	CA	ALA	A	315	18.609	110.124	51.841	1.00 99.77	A	C
ATOM	1683	CB	ALA	A	315	19.520	110.557	50.697	1.00103.35	A	C
ATOM	1684	C	ALA	A	315	17.696	108.990	51.389	1.00 96.97	A	C
ATOM	1685	O	ALA	A	315	17.904	107.837	51.755	1.00 97.14	A	O
ATOM	1686	N	MET	A	316	16.681	109.319	50.602	1.00 45.22	A	N
ATOM	1687	CA	MET	A	316	15.760	108.313	50.102	1.00 40.82	A	C
ATOM	1688	CB	MET	A	316	14.436	108.943	49.710	1.00 38.21	A	C
ATOM	1689	CG	MET	A	316	13.545	109.344	50.838	1.00 32.89	A	C
ATOM	1690	SD	MET	A	316	12.159	110.108	50.058	1.00 29.33	A	S
ATOM	1691	CE	MET	A	316	10.827	109.006	50.388	1.00 31.07	A	C
ATOM	1692	C	MET	A	316	16.348	107.689	48.859	1.00 39.34	A	C
ATOM	1693	O	MET	A	316	17.089	108.343	48.133	1.00 39.76	A	O
ATOM	1694	N	ALA	A	317	16.026	106.427	48.602	1.00 55.95	A	N
ATOM	1695	CA	ALA	A	317	16.517	105.783	47.392	1.00 53.74	A	C
ATOM	1696	CB	ALA	A	317	16.075	104.333	47.358	1.00107.40	A	C
ATOM	1697	C	ALA	A	317	15.850	106.578	46.267	1.00 51.31	A	C
ATOM	1698	O	ALA	A	317	14.802	107.182	46.487	1.00 51.08	A	O
ATOM	1699	N	ILE	A	318	16.434	106.597	45.074	1.00 26.23	A	N
ATOM	1700	CA	ILE	A	318	15.822	107.370	43.995	1.00 26.82	A	C
ATOM	1701	CB	ILE	A	318	16.527	107.185	42.652	1.00 43.92	A	C
ATOM	1702	CG2	ILE	A	318	15.609	107.613	41.533	1.00 43.98	A	C
ATOM	1703	CG1	ILE	A	318	17.775	108.051	42.581	1.00 44.78	A	C
ATOM	1704	CD1	ILE	A	318	18.450	107.976	41.223	1.00 46.89	A	C
ATOM	1705	C	ILE	A	318	14.356	107.064	43.751	1.00 25.98	A	C
ATOM	1706	O	ILE	A	318	13.522	107.966	43.724	1.00 25.78	A	O
ATOM	1707	N	PHE	A	319	14.018	105.801	43.549	1.00 38.81	A	N
ATOM	1708	CA	PHE	A	319	12.616	105.518	43.300	1.00 37.37	A	C
ATOM	1709	CB	PHE	A	319	12.399	104.039	42.979	1.00 29.42	A	C
ATOM	1710	CG	PHE	A	319	11.014	103.731	42.510	1.00 26.72	A	C
ATOM	1711	CD1	PHE	A	319	10.030	103.375	43.409	1.00 26.08	A	C
ATOM	1712	CD2	PHE	A	319	10.681	103.867	41.172	1.00 27.06	A	C
ATOM	1713	CE1	PHE	A	319	8.728	103.160	42.981	1.00 26.09	A	C
ATOM	1714	CE2	PHE	A	319	9.386	103.657	40.735	1.00 26.41	A	C

ATOM	1715	CZ	PHE	A	319	8.405	103.303	41.641	1.00	25.24	A	C
ATOM	1716	C	PHE	A	319	11.839	105.929	44.537	1.00	36.13	A	C
ATOM	1717	O	PHE	A	319	10.752	106.496	44.447	1.00	34.50	A	O
ATOM	1718	N	GLU	A	320	12.440	105.661	45.691	1.00	49.11	A	N
ATOM	1719	CA	GLU	A	320	11.858	105.995	46.984	1.00	50.67	A	C
ATOM	1720	CB	GLU	A	320	12.861	105.698	48.094	1.00	90.58	A	C
ATOM	1721	CG	GLU	A	320	12.283	105.715	49.488	1.00	94.98	A	C
ATOM	1722	CD	GLU	A	320	13.370	105.672	50.537	1.00	97.30	A	C
ATOM	1723	OE1	GLU	A	320	14.366	104.948	50.319	1.00	98.87	A	O
ATOM	1724	OE2	GLU	A	320	13.231	106.353	51.578	1.00	97.52	A	O
ATOM	1725	C	GLU	A	320	11.504	107.472	47.014	1.00	49.63	A	C
ATOM	1726	O	GLU	A	320	10.547	107.875	47.673	1.00	50.28	A	O
ATOM	1727	N	LEU	A	321	12.301	108.265	46.300	1.00	28.99	A	N
ATOM	1728	CA	LEU	A	321	12.115	109.712	46.194	1.00	28.04	A	C
ATOM	1729	CB	LEU	A	321	13.421	110.388	45.766	1.00	48.42	A	C
ATOM	1730	CG	LEU	A	321	13.296	111.908	45.680	1.00	48.69	A	C
ATOM	1731	CD1	LEU	A	321	13.611	112.412	47.061	1.00	48.76	A	C
ATOM	1732	CD2	LEU	A	321	14.230	112.548	44.646	1.00	48.06	A	C
ATOM	1733	C	LEU	A	321	11.038	110.049	45.160	1.00	26.11	A	C
ATOM	1734	O	LEU	A	321	9.951	110.509	45.506	1.00	23.10	A	O
ATOM	1735	N	LEU	A	322	11.368	109.820	43.888	1.00	40.80	A	N
ATOM	1736	CA	LEU	A	322	10.470	110.081	42.765	1.00	40.99	A	C
ATOM	1737	CB	LEU	A	322	10.948	109.326	41.531	1.00	14.45	A	C
ATOM	1738	CG	LEU	A	322	12.054	110.003	40.748	1.00	15.41	A	C
ATOM	1739	CD1	LEU	A	322	13.072	110.616	41.670	1.00	17.89	A	C
ATOM	1740	CD2	LEU	A	322	12.678	108.985	39.847	1.00	18.35	A	C
ATOM	1741	C	LEU	A	322	9.038	109.675	43.055	1.00	41.98	A	C
ATOM	1742	O	LEU	A	322	8.089	110.339	42.635	1.00	39.39	A	O
ATOM	1743	N	ASP	A	323	8.892	108.559	43.758	1.00	49.55	A	N
ATOM	1744	CA	ASP	A	323	7.580	108.061	44.101	1.00	50.42	A	C
ATOM	1745	CB	ASP	A	323	7.669	106.684	44.749	1.00	81.52	A	C
ATOM	1746	CG	ASP	A	323	6.376	105.916	44.633	1.00	84.22	A	C
ATOM	1747	OD1	ASP	A	323	6.186	104.919	45.362	1.00	86.08	A	O
ATOM	1748	OD2	ASP	A	323	5.550	106.316	43.791	1.00	83.63	A	O
ATOM	1749	C	ASP	A	323	7.009	109.039	45.092	1.00	50.69	A	C
ATOM	1750	O	ASP	A	323	5.897	109.520	44.931	1.00	51.43	A	O
ATOM	1751	N	TYR	A	324	7.785	109.344	46.120	1.00	50.92	A	N
ATOM	1752	CA	TYR	A	324	7.309	110.274	47.117	1.00	50.92	A	C
ATOM	1753	CB	TYR	A	324	8.451	110.795	47.987	1.00	63.45	A	C
ATOM	1754	CG	TYR	A	324	7.899	111.438	49.221	1.00	65.46	A	C
ATOM	1755	CD1	TYR	A	324	7.747	110.711	50.384	1.00	65.71	A	C
ATOM	1756	CE1	TYR	A	324	7.067	111.224	51.446	1.00	65.31	A	C
ATOM	1757	CD2	TYR	A	324	7.363	112.715	49.171	1.00	66.05	A	C

ATOM	1758	CE2	TYR	A	324	6.681	113.237	50.229	1.00	66.70	A	C
ATOM	1759	CZ	TYR	A	324	6.529	112.485	51.362	1.00	66.03	A	C
ATOM	1760	OH	TYR	A	324	5.784	112.977	52.401	1.00	67.67	A	O
ATOM	1761	C	TYR	A	324	6.632	111.452	46.424	1.00	50.82	A	C
ATOM	1762	O	TYR	A	324	5.464	111.747	46.672	1.00	49.49	A	O
ATOM	1763	N	ILE	A	325	7.380	112.104	45.544	1.00	49.82	A	N
ATOM	1764	CA	ILE	A	325	6.893	113.255	44.801	1.00	46.63	A	C
ATOM	1765	CB	ILE	A	325	7.895	113.703	43.779	1.00	11.84	A	C
ATOM	1766	CG2	ILE	A	325	7.236	114.697	42.844	1.00	13.93	A	C
ATOM	1767	CG1	ILE	A	325	9.126	114.281	44.468	1.00	10.61	A	C
ATOM	1768	CD1	ILE	A	325	10.195	114.726	43.498	1.00	10.40	A	C
ATOM	1769	C	ILE	A	325	5.589	113.087	44.039	1.00	47.94	A	C
ATOM	1770	O	ILE	A	325	4.614	113.775	44.311	1.00	48.37	A	O
ATOM	1771	N	VAL	A	326	5.584	112.205	43.057	1.00	31.50	A	N
ATOM	1772	CA	VAL	A	326	4.387	112.001	42.267	1.00	31.73	A	C
ATOM	1773	CB	VAL	A	326	4.653	111.032	41.110	1.00	41.65	A	C
ATOM	1774	CG1	VAL	A	326	5.556	111.689	40.103	1.00	39.85	A	C
ATOM	1775	CG2	VAL	A	326	5.324	109.789	41.619	1.00	42.38	A	C
ATOM	1776	C	VAL	A	326	3.222	111.505	43.104	1.00	34.52	A	C
ATOM	1777	O	VAL	A	326	2.284	112.263	43.351	1.00	35.65	A	O
ATOM	1778	N	ASN	A	327	3.293	110.252	43.547	1.00	51.08	A	N
ATOM	1779	CA	ASN	A	327	2.248	109.627	44.350	1.00	51.78	A	C
ATOM	1780	CB	ASN	A	327	2.784	108.368	45.021	1.00	155.81	A	C
ATOM	1781	CG	ASN	A	327	2.970	107.227	44.054	1.00	159.57	A	C
ATOM	1782	OD1	ASN	A	327	3.284	106.111	44.463	1.00	160.40	A	O
ATOM	1783	ND2	ASN	A	327	2.776	107.493	42.763	1.00	159.02	A	N
ATOM	1784	C	ASN	A	327	1.606	110.513	45.408	1.00	51.05	A	C
ATOM	1785	O	ASN	A	327	0.382	110.564	45.496	1.00	51.16	A	O
ATOM	1786	N	GLU	A	328	2.404	111.201	46.209	1.00	18.28	A	N
ATOM	1787	CA	GLU	A	328	1.839	112.069	47.240	1.00	17.66	A	C
ATOM	1788	CB	GLU	A	328	0.989	111.247	48.213	1.00	50.35	A	C
ATOM	1789	CG	GLU	A	328	1.571	111.139	49.644	1.00	50.42	A	C
ATOM	1790	CD	GLU	A	328	2.697	110.120	49.791	1.00	50.79	A	C
ATOM	1791	OE1	GLU	A	328	2.400	108.957	50.130	1.00	49.76	A	O
ATOM	1792	OE2	GLU	A	328	3.871	110.477	49.575	1.00	53.82	A	O
ATOM	1793	C	GLU	A	328	2.926	112.729	48.037	1.00	17.50	A	C
ATOM	1794	O	GLU	A	328	3.902	112.075	48.384	1.00	17.64	A	O
ATOM	1795	N	PRO	A	329	2.825	114.042	48.311	1.00	39.31	A	N
ATOM	1796	CD	PRO	A	329	3.050	113.915	49.751	1.00	68.50	A	C
ATOM	1797	CA	PRO	A	329	2.037	115.262	48.133	1.00	41.53	A	C
ATOM	1798	CB	PRO	A	329	1.062	115.222	49.316	1.00	69.37	A	C
ATOM	1799	CG	PRO	A	329	1.670	114.221	50.296	1.00	69.09	A	C
ATOM	1800	C	PRO	A	329	3.033	116.449	48.236	1.00	42.07	A	C

ATOM	1801	O	PRO	A	329	4.093	116.340	48.871	1.00	41.03	A	O
ATOM	1802	N	PRO	A	330	2.680	117.614	47.661	1.00	33.11	A	N
ATOM	1803	CD	PRO	A	330	1.328	118.041	47.264	1.00	57.29	A	C
ATOM	1804	CA	PRO	A	330	3.574	118.769	47.704	1.00	36.23	A	C
ATOM	1805	CB	PRO	A	330	2.778	119.838	46.978	1.00	57.89	A	C
ATOM	1806	CG	PRO	A	330	1.403	119.550	47.431	1.00	56.52	A	C
ATOM	1807	C	PRO	A	330	4.002	119.219	49.077	1.00	37.76	A	C
ATOM	1808	O	PRO	A	330	3.239	119.170	50.037	1.00	38.13	A	O
ATOM	1809	N	PRO	A	331	5.249	119.673	49.176	1.00	30.77	A	N
ATOM	1810	CD	PRO	A	331	6.199	119.643	48.054	1.00	36.99	A	C
ATOM	1811	CA	PRO	A	331	5.890	120.169	50.392	1.00	32.67	A	C
ATOM	1812	CB	PRO	A	331	7.367	120.112	50.042	1.00	38.05	A	C
ATOM	1813	CG	PRO	A	331	7.354	120.449	48.591	1.00	37.86	A	C
ATOM	1814	C	PRO	A	331	5.416	121.584	50.654	1.00	34.88	A	C
ATOM	1815	O	PRO	A	331	5.009	122.288	49.731	1.00	35.42	A	O
ATOM	1816	N	LYS	A	332	5.467	121.999	51.910	1.00	43.36	A	N
ATOM	1817	CA	LYS	A	332	5.030	123.333	52.284	1.00	43.81	A	C
ATOM	1818	CB	LYS	A	332	3.682	123.242	53.001	1.00	51.45	A	C
ATOM	1819	CG	LYS	A	332	3.584	122.044	53.918	1.00	53.34	A	C
ATOM	1820	CD	LYS	A	332	2.155	121.742	54.338	1.00	55.20	A	C
ATOM	1821	CE	LYS	A	332	2.096	120.437	55.151	1.00	53.90	A	C
ATOM	1822	NZ	LYS	A	332	0.717	120.028	55.573	1.00	54.05	A	N
ATOM	1823	C	LYS	A	332	6.070	123.990	53.176	1.00	44.24	A	C
ATOM	1824	O	LYS	A	332	7.074	123.370	53.528	1.00	45.01	A	O
ATOM	1825	N	LEU	A	333	5.842	125.251	53.525	1.00	52.24	A	N
ATOM	1826	CA	LEU	A	333	6.765	125.977	54.393	1.00	53.79	A	C
ATOM	1827	CB	LEU	A	333	6.810	127.465	54.016	1.00	35.39	A	C
ATOM	1828	CG	LEU	A	333	7.419	127.897	52.683	1.00	34.11	A	C
ATOM	1829	CD1	LEU	A	333	7.029	129.311	52.400	1.00	33.43	A	C
ATOM	1830	CD2	LEU	A	333	8.920	127.768	52.722	1.00	33.64	A	C
ATOM	1831	C	LEU	A	333	6.278	125.857	55.829	1.00	55.31	A	C
ATOM	1832	O	LEU	A	333	5.117	125.537	56.070	1.00	53.95	A	O
ATOM	1833	N	PRO	A	334	7.170	126.092	56.801	1.00	71.09	A	N
ATOM	1834	CD	PRO	A	334	8.627	126.210	56.638	1.00	98.35	A	C
ATOM	1835	CA	PRO	A	334	6.804	126.018	58.218	1.00	72.19	A	C
ATOM	1836	CB	PRO	A	334	8.124	126.294	58.922	1.00	98.14	A	C
ATOM	1837	CG	PRO	A	334	9.130	125.712	57.966	1.00	98.53	A	C
ATOM	1838	C	PRO	A	334	5.755	127.109	58.447	1.00	73.51	A	C
ATOM	1839	O	PRO	A	334	5.701	128.080	57.690	1.00	75.51	A	O
ATOM	1840	N	ASN	A	335	4.940	126.984	59.487	1.00	56.06	A	N
ATOM	1841	CA	ASN	A	335	3.871	127.951	59.680	1.00	55.87	A	C
ATOM	1842	CB	ASN	A	335	2.702	127.284	60.399	1.00	73.49	A	C
ATOM	1843	CG	ASN	A	335	1.362	127.820	59.933	1.00	74.92	A	C

ATOM	1844	OD1	ASN	A	335	1.119	127.947	58.732	1.00	76.33	A	O
ATOM	1845	ND2	ASN	A	335	0.483	128.129	60.878	1.00	74.05	A	N
ATOM	1846	C	ASN	A	335	4.141	129.305	60.311	1.00	55.03	A	C
ATOM	1847	O	ASN	A	335	4.390	130.269	59.606	1.00	54.64	A	O
ATOM	1848	N	GLY	A	336	4.072	129.399	61.629	1.00	53.63	A	N
ATOM	1849	CA	GLY	A	336	4.279	130.687	62.264	1.00	51.53	A	C
ATOM	1850	C	GLY	A	336	5.453	131.524	61.785	1.00	50.23	A	C
ATOM	1851	O	GLY	A	336	5.454	132.745	61.956	1.00	51.41	A	O
ATOM	1852	N	VAL	A	337	6.434	130.882	61.159	1.00	31.85	A	N
ATOM	1853	CA	VAL	A	337	7.652	131.558	60.704	1.00	31.02	A	C
ATOM	1854	CB	VAL	A	337	8.765	130.551	60.525	1.00	19.62	A	C
ATOM	1855	CG1	VAL	A	337	8.178	129.237	60.097	1.00	20.24	A	C
ATOM	1856	CG2	VAL	A	337	9.744	131.058	59.488	1.00	20.07	A	C
ATOM	1857	C	VAL	A	337	7.703	132.468	59.481	1.00	30.50	A	C
ATOM	1858	O	VAL	A	337	8.289	133.543	59.553	1.00	32.10	A	O
ATOM	1859	N	PHE	A	338	7.154	132.045	58.351	1.00	45.86	A	N
ATOM	1860	CA	PHE	A	338	7.199	132.895	57.161	1.00	44.46	A	C
ATOM	1861	CB	PHE	A	338	7.560	132.062	55.927	1.00	35.06	A	C
ATOM	1862	CG	PHE	A	338	8.868	131.323	56.058	1.00	31.81	A	C
ATOM	1863	CD1	PHE	A	338	10.070	131.939	55.759	1.00	32.06	A	C
ATOM	1864	CD2	PHE	A	338	8.892	130.008	56.489	1.00	29.92	A	C
ATOM	1865	CE1	PHE	A	338	11.274	131.248	55.886	1.00	32.87	A	C
ATOM	1866	CE2	PHE	A	338	10.084	129.324	56.615	1.00	29.00	A	C
ATOM	1867	CZ	PHE	A	338	11.272	129.943	56.314	1.00	30.66	A	C
ATOM	1868	C	PHE	A	338	5.872	133.622	56.951	1.00	45.14	A	C
ATOM	1869	O	PHE	A	338	4.830	133.193	57.440	1.00	46.65	A	O
ATOM	1870	N	THR	A	339	5.912	134.733	56.229	1.00	25.25	A	N
ATOM	1871	CA	THR	A	339	4.704	135.508	55.994	1.00	26.88	A	C
ATOM	1872	CB	THR	A	339	5.051	136.830	55.296	1.00	15.42	A	C
ATOM	1873	OG1	THR	A	339	5.729	136.580	54.063	1.00	18.04	A	O
ATOM	1874	CG2	THR	A	339	5.977	137.622	56.162	1.00	12.82	A	C
ATOM	1875	C	THR	A	339	3.662	134.725	55.200	1.00	27.11	A	C
ATOM	1876	O	THR	A	339	3.993	134.002	54.270	1.00	26.99	A	O
ATOM	1877	N	PRO	A	340	2.383	134.845	55.583	1.00	41.59	A	N
ATOM	1878	CD	PRO	A	340	1.953	135.490	56.834	1.00	24.23	A	C
ATOM	1879	CA	PRO	A	340	1.251	134.167	54.946	1.00	42.29	A	C
ATOM	1880	CB	PRO	A	340	0.051	134.718	55.703	1.00	26.51	A	C
ATOM	1881	CG	PRO	A	340	0.595	134.848	57.081	1.00	26.27	A	C
ATOM	1882	C	PRO	A	340	1.096	134.302	53.443	1.00	42.47	A	C
ATOM	1883	O	PRO	A	340	0.367	133.528	52.833	1.00	44.10	A	O
ATOM	1884	N	ASP	A	341	1.750	135.280	52.835	1.00	60.98	A	N
ATOM	1885	CA	ASP	A	341	1.646	135.413	51.393	1.00	62.37	A	C
ATOM	1886	CB	ASP	A	341	1.652	136.879	50.978	1.00	61.36	A	C

ATOM	1887	CG	ASP	A	341	0.305	137.525	51.163	1.00	61.94	A	C
ATOM	1888	OD1	ASP	A	341	-0.704	136.887	50.799	1.00	63.45	A	O
ATOM	1889	OD2	ASP	A	341	0.249	138.666	51.656	1.00	60.41	A	O
ATOM	1890	C	ASP	A	341	2.803	134.669	50.756	1.00	62.45	A	C
ATOM	1891	O	ASP	A	341	2.719	134.204	49.623	1.00	63.61	A	O
ATOM	1892	N	PHE	A	342	3.893	134.555	51.497	1.00	47.78	A	N
ATOM	1893	CA	PHE	A	342	5.047	133.828	51.007	1.00	46.75	A	C
ATOM	1894	CB	PHE	A	342	6.200	133.961	51.981	1.00	30.06	A	C
ATOM	1895	CG	PHE	A	342	7.412	133.191	51.590	1.00	29.99	A	C
ATOM	1896	CD1	PHE	A	342	7.978	133.357	50.349	1.00	30.65	A	C
ATOM	1897	CD2	PHE	A	342	8.026	132.360	52.492	1.00	30.43	A	C
ATOM	1898	CE1	PHE	A	342	9.131	132.721	50.016	1.00	32.11	A	C
ATOM	1899	CE2	PHE	A	342	9.182	131.720	52.162	1.00	30.02	A	C
ATOM	1900	CZ	PHE	A	342	9.737	131.904	50.918	1.00	31.65	A	C
ATOM	1901	C	PHE	A	342	4.624	132.379	50.937	1.00	45.40	A	C
ATOM	1902	O	PHE	A	342	4.924	131.680	49.974	1.00	45.36	A	O
ATOM	1903	N	GLN	A	343	3.929	131.938	51.982	1.00	24.69	A	N
ATOM	1904	CA	GLN	A	343	3.455	130.576	52.046	1.00	24.94	A	C
ATOM	1905	CB	GLN	A	343	2.723	130.304	53.352	1.00	63.15	A	C
ATOM	1906	CG	GLN	A	343	3.495	130.651	54.595	1.00	63.34	A	C
ATOM	1907	CD	GLN	A	343	2.816	130.132	55.845	1.00	64.04	A	C
ATOM	1908	OE1	GLN	A	343	3.090	130.594	56.952	1.00	64.23	A	O
ATOM	1909	NE2	GLN	A	343	1.930	129.156	55.677	1.00	64.68	A	N
ATOM	1910	C	GLN	A	343	2.492	130.433	50.902	1.00	24.42	A	C
ATOM	1911	O	GLN	A	343	2.586	129.494	50.128	1.00	25.51	A	O
ATOM	1912	N	GLU	A	344	1.571	131.380	50.782	1.00	26.30	A	N
ATOM	1913	CA	GLU	A	344	0.580	131.331	49.718	1.00	26.38	A	C
ATOM	1914	CB	GLU	A	344	-0.292	132.583	49.762	1.00	72.86	A	C
ATOM	1915	CG	GLU	A	344	-1.415	132.578	48.747	1.00	79.86	A	C
ATOM	1916	CD	GLU	A	344	-2.488	133.582	49.083	1.00	83.57	A	C
ATOM	1917	OE1	GLU	A	344	-3.504	133.631	48.361	1.00	84.94	A	O
ATOM	1918	OE2	GLU	A	344	-2.316	134.319	50.074	1.00	84.24	A	O
ATOM	1919	C	GLU	A	344	1.237	131.195	48.348	1.00	23.79	A	C
ATOM	1920	O	GLU	A	344	0.850	130.345	47.546	1.00	24.68	A	O
ATOM	1921	N	PHE	A	345	2.243	132.033	48.105	1.00	26.31	A	N
ATOM	1922	CA	PHE	A	345	3.008	132.060	46.860	1.00	23.73	A	C
ATOM	1923	CB	PHE	A	345	4.175	133.024	47.028	1.00	15.18	A	C
ATOM	1924	CG	PHE	A	345	4.975	133.233	45.787	1.00	13.30	A	C
ATOM	1925	CD1	PHE	A	345	4.380	133.757	44.651	1.00	12.42	A	C
ATOM	1926	CD2	PHE	A	345	6.328	132.921	45.753	1.00	13.51	A	C
ATOM	1927	CE1	PHE	A	345	5.119	133.967	43.495	1.00	11.32	A	C
ATOM	1928	CE2	PHE	A	345	7.073	133.127	44.607	1.00	14.83	A	C
ATOM	1929	CZ	PHE	A	345	6.465	133.652	43.471	1.00	12.81	A	C

ATOM	1930	C	PHE	A	345	3.538	130.674	46.508	1.00	24.04	A	C
ATOM	1931	O	PHE	A	345	3.179	130.098	45.484	1.00	23.31	A	O
ATOM	1932	N	VAL	A	346	4.390	130.155	47.389	1.00	40.87	A	N
ATOM	1933	CA	VAL	A	346	5.023	128.848	47.246	1.00	41.14	A	C
ATOM	1934	CB	VAL	A	346	5.913	128.559	48.458	1.00	32.63	A	C
ATOM	1935	CG1	VAL	A	346	6.543	127.209	48.316	1.00	34.30	A	C
ATOM	1936	CG2	VAL	A	346	6.983	129.612	48.572	1.00	34.08	A	C
ATOM	1937	C	VAL	A	346	4.044	127.686	47.074	1.00	41.37	A	C
ATOM	1938	O	VAL	A	346	4.309	126.721	46.345	1.00	42.54	A	O
ATOM	1939	N	ASN	A	347	2.911	127.778	47.750	1.00	20.79	A	N
ATOM	1940	CA	ASN	A	347	1.910	126.742	47.655	1.00	22.04	A	C
ATOM	1941	CB	ASN	A	347	0.833	126.982	48.689	1.00	38.04	A	C
ATOM	1942	CG	ASN	A	347	1.272	126.598	50.082	1.00	38.10	A	C
ATOM	1943	OD1	ASN	A	347	2.431	126.757	50.461	1.00	35.13	A	O
ATOM	1944	ND2	ASN	A	347	0.334	126.100	50.861	1.00	39.71	A	N
ATOM	1945	C	ASN	A	347	1.296	126.713	46.270	1.00	22.73	A	C
ATOM	1946	O	ASN	A	347	0.878	125.655	45.802	1.00	23.98	A	O
ATOM	1947	N	LYS	A	348	1.237	127.871	45.611	1.00	31.92	A	N
ATOM	1948	CA	LYS	A	348	0.670	127.949	44.262	1.00	34.81	A	C
ATOM	1949	CB	LYS	A	348	0.328	129.400	43.902	1.00	48.25	A	C
ATOM	1950	CG	LYS	A	348	-0.990	129.875	44.513	1.00	51.16	A	C
ATOM	1951	CD	LYS	A	348	-1.216	131.387	44.364	1.00	53.88	A	C
ATOM	1952	CE	LYS	A	348	-2.399	131.855	45.230	1.00	56.96	A	C
ATOM	1953	NZ	LYS	A	348	-2.583	133.336	45.293	1.00	56.97	A	N
ATOM	1954	C	LYS	A	348	1.612	127.350	43.227	1.00	34.92	A	C
ATOM	1955	O	LYS	A	348	1.169	126.748	42.258	1.00	35.41	A	O
ATOM	1956	N	CYS	A	349	2.912	127.513	43.446	1.00	45.78	A	N
ATOM	1957	CA	CYS	A	349	3.908	126.962	42.540	1.00	43.77	A	C
ATOM	1958	CB	CYS	A	349	5.303	127.485	42.855	1.00	22.22	A	C
ATOM	1959	SG	CYS	A	349	5.444	129.236	43.020	1.00	22.51	A	S
ATOM	1960	C	CYS	A	349	3.936	125.466	42.747	1.00	44.23	A	C
ATOM	1961	O	CYS	A	349	3.964	124.696	41.787	1.00	45.92	A	O
ATOM	1962	N	LEU	A	350	3.943	125.062	44.015	1.00	50.11	A	N
ATOM	1963	CA	LEU	A	350	3.994	123.653	44.356	1.00	50.75	A	C
ATOM	1964	CB	LEU	A	350	4.752	123.458	45.668	1.00	7.57	A	C
ATOM	1965	CG	LEU	A	350	6.249	123.770	45.677	1.00	7.57	A	C
ATOM	1966	CD1	LEU	A	350	6.794	123.686	47.110	1.00	7.07	A	C
ATOM	1967	CD2	LEU	A	350	6.977	122.807	44.769	1.00	6.39	A	C
ATOM	1968	C	LEU	A	350	2.633	122.967	44.436	1.00	51.76	A	C
ATOM	1969	O	LEU	A	350	2.217	122.513	45.495	1.00	53.73	A	O
ATOM	1970	N	ILE	A	351	1.941	122.898	43.307	1.00	12.84	A	N
ATOM	1971	CA	ILE	A	351	0.651	122.231	43.225	1.00	13.77	A	C
ATOM	1972	CB	ILE	A	351	-0.422	123.151	42.650	1.00	17.52	A	C

ATOM	1973	CG2	ILE	A	351	-1.667	122.371	42.310	1.00 16.89	A	C
ATOM	1974	CG1	ILE	A	351	-0.738	124.254	43.643	1.00 15.78	A	C
ATOM	1975	CD1	ILE	A	351	-1.964	124.984	43.269	1.00 16.88	A	C
ATOM	1976	C	ILE	A	351	0.868	121.094	42.255	1.00 15.06	A	C
ATOM	1977	O	ILE	A	351	1.203	121.340	41.103	1.00 16.03	A	O
ATOM	1978	N	LYS	A	352	0.677	119.856	42.703	1.00 64.60	A	N
ATOM	1979	CA	LYS	A	352	0.909	118.703	41.837	1.00 65.04	A	C
ATOM	1980	CB	LYS	A	352	0.568	117.411	42.579	1.00 65.12	A	C
ATOM	1981	CG	LYS	A	352	1.485	117.192	43.780	1.00 65.43	A	C
ATOM	1982	CD	LYS	A	352	1.715	115.721	44.108	1.00 63.18	A	C
ATOM	1983	CE	LYS	A	352	0.429	115.028	44.504	1.00 62.06	A	C
ATOM	1984	NZ	LYS	A	352	0.649	113.604	44.870	1.00 62.44	A	N
ATOM	1985	C	LYS	A	352	0.212	118.767	40.481	1.00 65.93	A	C
ATOM	1986	O	LYS	A	352	0.813	118.456	39.453	1.00 66.96	A	O
ATOM	1987	N	ASN	A	353	-1.051	119.163	40.460	1.00 27.97	A	N
ATOM	1988	CA	ASN	A	353	-1.717	119.287	39.179	1.00 28.91	A	C
ATOM	1989	CB	ASN	A	353	-3.209	119.516	39.323	1.00 32.32	A	C
ATOM	1990	CG	ASN	A	353	-3.846	119.819	37.999	1.00 30.87	A	C
ATOM	1991	OD1	ASN	A	353	-3.155	120.184	37.051	1.00 27.07	A	O
ATOM	1992	ND2	ASN	A	353	-5.159	119.675	37.915	1.00 33.42	A	N
ATOM	1993	C	ASN	A	353	-1.123	120.507	38.503	1.00 28.36	A	C
ATOM	1994	O	ASN	A	353	-1.255	121.635	38.984	1.00 27.72	A	O
ATOM	1995	N	PRO	A	354	-0.487	120.306	37.358	1.00 22.90	A	N
ATOM	1996	CD	PRO	A	354	-0.471	119.095	36.530	1.00 23.51	A	C
ATOM	1997	CA	PRO	A	354	0.117	121.419	36.649	1.00 22.52	A	C
ATOM	1998	CB	PRO	A	354	0.835	120.732	35.511	1.00 23.78	A	C
ATOM	1999	CG	PRO	A	354	-0.118	119.645	35.168	1.00 24.60	A	C
ATOM	2000	C	PRO	A	354	-0.938	122.351	36.134	1.00 22.17	A	C
ATOM	2001	O	PRO	A	354	-0.742	123.560	36.090	1.00 21.55	A	O
ATOM	2002	N	ALA	A	355	-2.062	121.766	35.746	1.00 24.27	A	N
ATOM	2003	CA	ALA	A	355	-3.168	122.502	35.158	1.00 26.32	A	C
ATOM	2004	CB	ALA	A	355	-4.159	121.530	34.536	1.00127.21	A	C
ATOM	2005	C	ALA	A	355	-3.907	123.473	36.036	1.00 26.06	A	C
ATOM	2006	O	ALA	A	355	-4.712	124.243	35.536	1.00 25.57	A	O
ATOM	2007	N	GLU	A	356	-3.669	123.458	37.336	1.00 70.69	A	N
ATOM	2008	CA	GLU	A	356	-4.392	124.409	38.155	1.00 71.73	A	C
ATOM	2009	CB	GLU	A	356	-5.486	123.706	38.958	1.00 74.31	A	C
ATOM	2010	CG	GLU	A	356	-5.020	122.970	40.171	1.00 81.06	A	C
ATOM	2011	CD	GLU	A	356	-6.188	122.441	40.967	1.00 83.85	A	C
ATOM	2012	OE1	GLU	A	356	-5.965	121.889	42.066	1.00 84.92	A	O
ATOM	2013	OE2	GLU	A	356	-7.335	122.579	40.489	1.00 83.88	A	O
ATOM	2014	C	GLU	A	356	-3.477	125.202	39.066	1.00 71.37	A	C
ATOM	2015	O	GLU	A	356	-3.929	125.963	39.920	1.00 70.05	A	O

ATOM	2016	N	ARG	A	357	-2.181	125.040	38.862	1.00	38.87	A	N
ATOM	2017	CA	ARG	A	357	-1.217	125.754	39.661	1.00	37.08	A	C
ATOM	2018	CB	ARG	A	357	0.036	124.908	39.835	1.00	32.03	A	C
ATOM	2019	CG	ARG	A	357	1.283	125.435	39.181	1.00	27.34	A	C
ATOM	2020	CD	ARG	A	357	2.398	124.463	39.445	1.00	26.49	A	C
ATOM	2021	NE	ARG	A	357	2.079	123.138	38.914	1.00	24.34	A	N
ATOM	2022	CZ	ARG	A	357	2.856	122.068	39.053	1.00	22.58	A	C
ATOM	2023	NH1	ARG	A	357	3.994	122.172	39.714	1.00	21.55	A	N
ATOM	2024	NH2	ARG	A	357	2.511	120.903	38.521	1.00	21.62	A	N
ATOM	2025	C	ARG	A	357	-0.872	127.062	38.987	1.00	36.31	A	C
ATOM	2026	O	ARG	A	357	-1.148	127.260	37.804	1.00	36.68	A	O
ATOM	2027	N	ALA	A	358	-0.261	127.952	39.755	1.00	27.23	A	N
ATOM	2028	CA	ALA	A	358	0.138	129.268	39.281	1.00	26.92	A	C
ATOM	2029	CB	ALA	A	358	0.958	129.953	40.353	1.00	24.81	A	C
ATOM	2030	C	ALA	A	358	0.917	129.276	37.984	1.00	27.40	A	C
ATOM	2031	O	ALA	A	358	1.812	128.466	37.782	1.00	28.30	A	O
ATOM	2032	N	ASP	A	359	0.567	130.202	37.102	1.00	26.78	A	N
ATOM	2033	CA	ASP	A	359	1.288	130.362	35.849	1.00	26.91	A	C
ATOM	2034	CB	ASP	A	359	0.347	130.675	34.696	1.00	53.41	A	C
ATOM	2035	CG	ASP	A	359	-0.236	132.063	34.795	1.00	52.77	A	C
ATOM	2036	OD1	ASP	A	359	-1.219	132.241	35.544	1.00	48.93	A	O
ATOM	2037	OD2	ASP	A	359	0.302	132.980	34.136	1.00	53.95	A	O
ATOM	2038	C	ASP	A	359	2.117	131.595	36.157	1.00	26.48	A	C
ATOM	2039	O	ASP	A	359	1.974	132.171	37.237	1.00	24.84	A	O
ATOM	2040	N	LEU	A	360	2.958	132.017	35.217	1.00	27.98	A	N
ATOM	2041	CA	LEU	A	360	3.817	133.178	35.432	1.00	26.03	A	C
ATOM	2042	CB	LEU	A	360	4.720	133.398	34.218	1.00	14.79	A	C
ATOM	2043	CG	LEU	A	360	5.803	132.321	34.079	1.00	13.54	A	C
ATOM	2044	CD1	LEU	A	360	6.638	132.552	32.836	1.00	12.21	A	C
ATOM	2045	CD2	LEU	A	360	6.685	132.335	35.301	1.00	14.39	A	C
ATOM	2046	C	LEU	A	360	3.081	134.457	35.797	1.00	24.70	A	C
ATOM	2047	O	LEU	A	360	3.665	135.361	36.394	1.00	24.33	A	O
ATOM	2048	N	LYS	A	361	1.797	134.523	35.470	1.00	22.05	A	N
ATOM	2049	CA	LYS	A	361	0.999	135.705	35.791	1.00	24.77	A	C
ATOM	2050	CB	LYS	A	361	-0.284	135.726	34.970	1.00	61.70	A	C
ATOM	2051	CG	LYS	A	361	-1.271	136.757	35.467	1.00	60.64	A	C
ATOM	2052	CD	LYS	A	361	-1.459	137.874	34.469	1.00	59.82	A	C
ATOM	2053	CE	LYS	A	361	-2.202	137.380	33.247	1.00	58.71	A	C
ATOM	2054	NZ	LYS	A	361	-2.447	138.487	32.292	1.00	61.68	A	N
ATOM	2055	C	LYS	A	361	0.637	135.831	37.273	1.00	26.20	A	C
ATOM	2056	O	LYS	A	361	1.113	136.750	37.944	1.00	26.16	A	O
ATOM	2057	N	MET	A	362	-0.206	134.925	37.779	1.00	25.24	A	N
ATOM	2058	CA	MET	A	362	-0.614	134.957	39.188	1.00	26.30	A	C

ATOM	2059	CB	MET	A	362	-1.198	133.610	39.656	1.00	70.42	A	C
ATOM	2060	CG	MET	A	362	-2.600	133.285	39.175	1.00	75.52	A	C
ATOM	2061	SD	MET	A	362	-2.652	132.165	37.761	1.00	81.47	A	S
ATOM	2062	CE	MET	A	362	-2.954	130.596	38.586	1.00	81.28	A	C
ATOM	2063	C	MET	A	362	0.607	135.245	40.029	1.00	25.24	A	C
ATOM	2064	O	MET	A	362	0.649	136.168	40.839	1.00	25.21	A	O
ATOM	2065	N	LEU	A	363	1.613	134.425	39.817	1.00	21.47	A	N
ATOM	2066	CA	LEU	A	363	2.830	134.567	40.554	1.00	21.24	A	C
ATOM	2067	CB	LEU	A	363	3.837	133.534	40.080	1.00	29.74	A	C
ATOM	2068	CG	LEU	A	363	3.470	132.110	40.450	1.00	29.05	A	C
ATOM	2069	CD1	LEU	A	363	4.758	131.320	40.482	1.00	29.06	A	C
ATOM	2070	CD2	LEU	A	363	2.782	132.058	41.806	1.00	26.46	A	C
ATOM	2071	C	LEU	A	363	3.426	135.942	40.428	1.00	20.17	A	C
ATOM	2072	O	LEU	A	363	3.705	136.603	41.429	1.00	20.62	A	O
ATOM	2073	N	THR	A	364	3.626	136.366	39.190	1.00	10.32	A	N
ATOM	2074	CA	THR	A	364	4.241	137.644	38.940	1.00	10.90	A	C
ATOM	2075	CB	THR	A	364	4.453	137.819	37.456	1.00	27.33	A	C
ATOM	2076	OG1	THR	A	364	5.836	138.126	37.211	1.00	26.24	A	O
ATOM	2077	CG2	THR	A	364	3.556	138.911	36.926	1.00	29.11	A	C
ATOM	2078	C	THR	A	364	3.485	138.828	39.551	1.00	10.41	A	C
ATOM	2079	O	THR	A	364	4.047	139.908	39.770	1.00	11.18	A	O
ATOM	2080	N	ASN	A	365	2.213	138.627	39.855	1.00	21.74	A	N
ATOM	2081	CA	ASN	A	365	1.456	139.689	40.483	1.00	20.59	A	C
ATOM	2082	CB	ASN	A	365	0.231	140.030	39.643	1.00	56.73	A	C
ATOM	2083	CG	ASN	A	365	0.605	140.645	38.317	1.00	59.50	A	C
ATOM	2084	OD1	ASN	A	365	1.416	141.567	38.259	1.00	63.75	A	O
ATOM	2085	ND2	ASN	A	365	0.017	140.143	37.242	1.00	60.94	A	N
ATOM	2086	C	ASN	A	365	1.050	139.281	41.894	1.00	19.27	A	C
ATOM	2087	O	ASN	A	365	0.257	139.952	42.540	1.00	20.31	A	O
ATOM	2088	N	HIS	A	366	1.603	138.177	42.384	1.00	33.33	A	N
ATOM	2089	CA	HIS	A	366	1.258	137.728	43.724	1.00	32.13	A	C
ATOM	2090	CB	HIS	A	366	2.040	136.484	44.138	1.00	25.48	A	C
ATOM	2091	CG	HIS	A	366	1.549	135.897	45.418	1.00	24.78	A	C
ATOM	2092	CD2	HIS	A	366	1.747	136.276	46.700	1.00	24.06	A	C
ATOM	2093	ND1	HIS	A	366	0.610	134.890	45.460	1.00	26.20	A	N
ATOM	2094	CE1	HIS	A	366	0.242	134.682	46.710	1.00	26.38	A	C
ATOM	2095	NE2	HIS	A	366	0.918	135.512	47.483	1.00	25.72	A	N
ATOM	2096	C	HIS	A	366	1.563	138.832	44.705	1.00	29.66	A	C
ATOM	2097	O	HIS	A	366	2.600	139.473	44.625	1.00	28.49	A	O
ATOM	2098	N	THR	A	367	0.658	139.048	45.642	1.00	38.52	A	N
ATOM	2099	CA	THR	A	367	0.845	140.096	46.625	1.00	38.52	A	C
ATOM	2100	CB	THR	A	367	-0.277	140.036	47.677	1.00	27.85	A	C
ATOM	2101	OG1	THR	A	367	-0.343	141.273	48.385	1.00	28.85	A	O

ATOM	2102	CG2	THR	A	367	-0.019	138.932	48.650	1.00	28.92	A	C
ATOM	2103	C	THR	A	367	2.226	140.005	47.298	1.00	37.37	A	C
ATOM	2104	O	THR	A	367	2.698	140.971	47.889	1.00	38.03	A	O
ATOM	2105	N	PHE	A	368	2.882	138.855	47.172	1.00	15.68	A	N
ATOM	2106	CA	PHE	A	368	4.204	138.624	47.770	1.00	16.25	A	C
ATOM	2107	CB	PHE	A	368	4.441	137.106	47.918	1.00	28.85	A	C
ATOM	2108	CG	PHE	A	368	5.880	136.719	48.101	1.00	26.40	A	C
ATOM	2109	CD1	PHE	A	368	6.541	136.965	49.295	1.00	26.51	A	C
ATOM	2110	CD2	PHE	A	368	6.588	136.135	47.058	1.00	25.60	A	C
ATOM	2111	CE1	PHE	A	368	7.890	136.639	49.443	1.00	26.85	A	C
ATOM	2112	CE2	PHE	A	368	7.938	135.805	47.200	1.00	25.60	A	C
ATOM	2113	CZ	PHE	A	368	8.585	136.061	48.393	1.00	25.60	A	C
ATOM	2114	C	PHE	A	368	5.317	139.269	46.950	1.00	15.34	A	C
ATOM	2115	O	PHE	A	368	6.228	139.878	47.500	1.00	13.15	A	O
ATOM	2116	N	ILE	A	369	5.230	139.123	45.630	1.00	11.11	A	N
ATOM	2117	CA	ILE	A	369	6.200	139.691	44.694	1.00	14.50	A	C
ATOM	2118	CB	ILE	A	369	5.959	139.207	43.246	1.00	30.14	A	C
ATOM	2119	CG2	ILE	A	369	6.917	139.901	42.312	1.00	28.77	A	C
ATOM	2120	CG1	ILE	A	369	6.146	137.697	43.159	1.00	30.02	A	C
ATOM	2121	CD1	ILE	A	369	7.492	137.262	43.662	1.00	32.00	A	C
ATOM	2122	C	ILE	A	369	6.053	141.194	44.693	1.00	16.88	A	C
ATOM	2123	O	ILE	A	369	7.027	141.916	44.486	1.00	17.69	A	O
ATOM	2124	N	LYS	A	370	4.813	141.644	44.899	1.00	27.85	A	N
ATOM	2125	CA	LYS	A	370	4.475	143.061	44.957	1.00	29.79	A	C
ATOM	2126	CB	LYS	A	370	2.959	143.243	45.053	1.00	67.59	A	C
ATOM	2127	CG	LYS	A	370	2.228	143.219	43.713	1.00	70.53	A	C
ATOM	2128	CD	LYS	A	370	0.702	143.227	43.896	1.00	75.21	A	C
ATOM	2129	CE	LYS	A	370	0.192	144.404	44.744	1.00	76.93	A	C
ATOM	2130	NZ	LYS	A	370	0.313	145.743	44.082	1.00	77.89	A	N
ATOM	2131	C	LYS	A	370	5.151	143.660	46.184	1.00	29.70	A	C
ATOM	2132	O	LYS	A	370	5.976	144.558	46.072	1.00	28.22	A	O
ATOM	2133	N	ARG	A	371	4.790	143.160	47.357	1.00	15.97	A	N
ATOM	2134	CA	ARG	A	371	5.387	143.616	48.601	1.00	15.89	A	C
ATOM	2135	CB	ARG	A	371	5.107	142.573	49.679	1.00	40.64	A	C
ATOM	2136	CG	ARG	A	371	5.261	143.002	51.114	1.00	40.29	A	C
ATOM	2137	CD	ARG	A	371	5.047	141.783	52.005	1.00	40.41	A	C
ATOM	2138	NE	ARG	A	371	6.227	140.912	51.985	1.00	39.64	A	N
ATOM	2139	CZ	ARG	A	371	6.234	139.592	52.186	1.00	37.69	A	C
ATOM	2140	NH1	ARG	A	371	5.109	138.923	52.423	1.00	36.14	A	N
ATOM	2141	NH2	ARG	A	371	7.391	138.942	52.161	1.00	36.41	A	N
ATOM	2142	C	ARG	A	371	6.883	143.673	48.316	1.00	15.29	A	C
ATOM	2143	O	ARG	A	371	7.561	144.667	48.555	1.00	15.42	A	O
ATOM	2144	N	SER	A	372	7.375	142.581	47.755	1.00	40.79	A	N

ATOM	2145	CA	SER	A	372	8.779	142.417	47.434	1.00	44.14	A	C
ATOM	2146	CB	SER	A	372	8.982	141.060	46.757	1.00	39.16	A	C
ATOM	2147	OG	SER	A	372	8.706	139.999	47.657	1.00	39.94	A	O
ATOM	2148	C	SER	A	372	9.413	143.512	46.591	1.00	46.18	A	C
ATOM	2149	O	SER	A	372	10.464	144.027	46.934	1.00	46.43	A	O
ATOM	2150	N	GLU	A	373	8.792	143.865	45.479	1.00	53.20	A	N
ATOM	2151	CA	GLU	A	373	9.368	144.888	44.621	1.00	54.19	A	C
ATOM	2152	CB	GLU	A	373	8.570	144.976	43.329	1.00	40.00	A	C
ATOM	2153	CG	GLU	A	373	8.526	143.693	42.551	1.00	44.22	A	C
ATOM	2154	CD	GLU	A	373	7.449	143.714	41.501	1.00	47.00	A	C
ATOM	2155	OE1	GLU	A	373	7.467	142.839	40.609	1.00	49.04	A	O
ATOM	2156	OE2	GLU	A	373	6.575	144.602	41.570	1.00	46.91	A	O
ATOM	2157	C	GLU	A	373	9.389	146.248	45.301	1.00	53.99	A	C
ATOM	2158	O	GLU	A	373	10.063	147.176	44.852	1.00	53.28	A	O
ATOM	2159	N	VAL	A	374	8.661	146.355	46.402	1.00	44.45	A	N
ATOM	2160	CA	VAL	A	374	8.569	147.615	47.116	1.00	45.54	A	C
ATOM	2161	CB	VAL	A	374	7.187	147.736	47.797	1.00	21.85	A	C
ATOM	2162	CG1	VAL	A	374	6.964	149.133	48.330	1.00	21.24	A	C
ATOM	2163	CG2	VAL	A	374	6.124	147.395	46.807	1.00	20.37	A	C
ATOM	2164	C	VAL	A	374	9.660	147.823	48.150	1.00	44.46	A	C
ATOM	2165	O	VAL	A	374	10.253	148.896	48.209	1.00	46.04	A	O
ATOM	2166	N	GLU	A	375	9.935	146.798	48.953	1.00	34.81	A	N
ATOM	2167	CA	GLU	A	375	10.936	146.912	50.007	1.00	34.94	A	C
ATOM	2168	CB	GLU	A	375	10.900	145.670	50.904	1.00	140.12	A	C
ATOM	2169	CG	GLU	A	375	11.954	145.648	52.021	1.00	134.14	A	C
ATOM	2170	CD	GLU	A	375	11.954	146.893	52.919	1.00	128.86	A	C
ATOM	2171	OE1	GLU	A	375	12.672	146.869	53.945	1.00	129.22	A	O
ATOM	2172	OE2	GLU	A	375	11.256	147.889	52.608	1.00	127.22	A	O
ATOM	2173	C	GLU	A	375	12.363	147.177	49.552	1.00	36.57	A	C
ATOM	2174	O	GLU	A	375	12.725	146.908	48.419	1.00	36.94	A	O
ATOM	2175	N	GLU	A	376	13.154	147.755	50.452	1.00	51.96	A	N
ATOM	2176	CA	GLU	A	376	14.552	148.045	50.187	1.00	54.71	A	C
ATOM	2177	CB	GLU	A	376	14.992	149.333	50.905	1.00	203.67	A	C
ATOM	2178	CG	GLU	A	376	14.514	149.456	52.358	1.00	203.67	A	C
ATOM	2179	CD	GLU	A	376	15.269	150.513	53.159	1.00	203.67	A	C
ATOM	2180	OE1	GLU	A	376	16.407	150.232	53.595	1.00	203.67	A	O
ATOM	2181	OE2	GLU	A	376	14.723	151.623	53.347	1.00	203.67	A	O
ATOM	2182	C	GLU	A	376	15.333	146.861	50.728	1.00	55.81	A	C
ATOM	2183	O	GLU	A	376	15.566	146.767	51.931	1.00	57.62	A	O
ATOM	2184	N	VAL	A	377	15.712	145.937	49.857	1.00	83.31	A	N
ATOM	2185	CA	VAL	A	377	16.476	144.780	50.313	1.00	85.22	A	C
ATOM	2186	CB	VAL	A	377	15.844	143.436	49.864	1.00	107.94	A	C
ATOM	2187	CG1	VAL	A	377	16.083	142.366	50.922	1.00	107.24	A	C

ATOM	2188	CG2	VAL	A	377	14.369	143.610	49.592	1.00	106.74	A	C
ATOM	2189	C	VAL	A	377	17.846	144.886	49.671	1.00	85.66	A	C
ATOM	2190	O	VAL	A	377	17.969	144.809	48.445	1.00	85.34	A	O
ATOM	2191	N	ASP	A	378	18.879	145.071	50.481	1.00	59.00	A	N
ATOM	2192	CA	ASP	A	378	20.216	145.179	49.936	1.00	59.40	A	C
ATOM	2193	CB	ASP	A	378	21.122	145.893	50.933	1.00	41.87	A	C
ATOM	2194	CG	ASP	A	378	22.507	146.156	50.390	1.00	38.94	A	C
ATOM	2195	OD1	ASP	A	378	23.371	146.584	51.175	1.00	37.73	A	O
ATOM	2196	OD2	ASP	A	378	22.732	145.938	49.181	1.00	36.31	A	O
ATOM	2197	C	ASP	A	378	20.764	143.784	49.638	1.00	61.15	A	C
ATOM	2198	O	ASP	A	378	21.470	143.207	50.466	1.00	63.19	A	O
ATOM	2199	N	PHE	A	379	20.432	143.232	48.462	1.00	76.82	A	N
ATOM	2200	CA	PHE	A	379	20.919	141.904	48.100	1.00	75.79	A	C
ATOM	2201	CB	PHE	A	379	20.265	141.370	46.813	1.00	40.93	A	C
ATOM	2202	CG	PHE	A	379	20.782	140.016	46.395	1.00	40.05	A	C
ATOM	2203	CD1	PHE	A	379	21.978	139.900	45.705	1.00	40.60	A	C
ATOM	2204	CD2	PHE	A	379	20.135	138.861	46.793	1.00	38.49	A	C
ATOM	2205	CE1	PHE	A	379	22.519	138.662	45.424	1.00	40.10	A	C
ATOM	2206	CE2	PHE	A	379	20.674	137.630	46.515	1.00	37.47	A	C
ATOM	2207	CZ	PHE	A	379	21.871	137.532	45.828	1.00	38.18	A	C
ATOM	2208	C	PHE	A	379	22.428	141.936	47.919	1.00	75.49	A	C
ATOM	2209	O	PHE	A	379	23.117	140.972	48.246	1.00	75.96	A	O
ATOM	2210	N	ALA	A	380	22.929	143.046	47.389	1.00	50.73	A	N
ATOM	2211	CA	ALA	A	380	24.361	143.201	47.188	1.00	52.48	A	C
ATOM	2212	CB	ALA	A	380	24.655	144.552	46.566	1.00	91.86	A	C
ATOM	2213	C	ALA	A	380	24.979	143.110	48.573	1.00	52.93	A	C
ATOM	2214	O	ALA	A	380	25.871	142.289	48.823	1.00	51.50	A	O
ATOM	2215	N	GLY	A	381	24.476	143.949	49.473	1.00	45.14	A	N
ATOM	2216	CA	GLY	A	381	24.966	143.962	50.835	1.00	46.97	A	C
ATOM	2217	C	GLY	A	381	24.909	142.584	51.459	1.00	48.85	A	C
ATOM	2218	O	GLY	A	381	25.943	141.949	51.656	1.00	49.66	A	O
ATOM	2219	N	TRP	A	382	23.703	142.110	51.764	1.00	43.15	A	N
ATOM	2220	CA	TRP	A	382	23.535	140.797	52.375	1.00	42.26	A	C
ATOM	2221	CB	TRP	A	382	22.086	140.336	52.326	1.00	54.96	A	C
ATOM	2222	CG	TRP	A	382	21.964	138.893	52.734	1.00	54.92	A	C
ATOM	2223	CD2	TRP	A	382	22.011	137.744	51.871	1.00	54.89	A	C
ATOM	2224	CE2	TRP	A	382	21.967	136.602	52.691	1.00	55.62	A	C
ATOM	2225	CE3	TRP	A	382	22.088	137.573	50.483	1.00	54.54	A	C
ATOM	2226	CD1	TRP	A	382	21.890	138.408	54.002	1.00	55.75	A	C
ATOM	2227	NE1	TRP	A	382	21.894	137.035	53.988	1.00	55.73	A	N
ATOM	2228	CZ2	TRP	A	382	22.002	135.306	52.173	1.00	55.36	A	C
ATOM	2229	CZ3	TRP	A	382	22.123	136.284	49.972	1.00	55.38	A	C
ATOM	2230	CH2	TRP	A	382	22.079	135.169	50.816	1.00	55.83	A	C

ATOM	2231	C	TRP	A	382	24.358	139.694	51.745	1.00 42.31	A	C
ATOM	2232	O	TRP	A	382	24.861	138.829	52.449	1.00 42.68	A	O
ATOM	2233	N	LEU	A	383	24.474	139.702	50.421	1.00 53.39	A	N
ATOM	2234	CA	LEU	A	383	25.211	138.651	49.728	1.00 55.83	A	C
ATOM	2235	CB	LEU	A	383	25.152	138.842	48.216	1.00 44.38	A	C
ATOM	2236	CG	LEU	A	383	25.743	137.657	47.452	1.00 44.54	A	C
ATOM	2237	CD1	LEU	A	383	24.847	136.447	47.613	1.00 44.55	A	C
ATOM	2238	CD2	LEU	A	383	25.882	138.009	45.998	1.00 43.21	A	C
ATOM	2239	C	LEU	A	383	26.658	138.572	50.146	1.00 57.21	A	C
ATOM	2240	O	LEU	A	383	27.251	137.498	50.134	1.00 55.74	A	O
ATOM	2241	N	CYS	A	384	27.231	139.713	50.504	1.00 59.50	A	N
ATOM	2242	CA	CYS	A	384	28.626	139.771	50.931	1.00 60.36	A	C
ATOM	2243	CB	CYS	A	384	29.230	141.094	50.476	1.00 46.87	A	C
ATOM	2244	SG	CYS	A	384	28.568	141.628	48.883	1.00 48.73	A	S
ATOM	2245	C	CYS	A	384	28.702	139.635	52.453	1.00 61.86	A	C
ATOM	2246	O	CYS	A	384	29.606	138.998	52.984	1.00 61.41	A	O
ATOM	2247	N	LYS	A	385	27.740	140.233	53.147	1.00 94.97	A	N
ATOM	2248	CA	LYS	A	385	27.683	140.153	54.602	1.00 96.00	A	C
ATOM	2249	CB	LYS	A	385	26.414	140.846	55.113	1.00172.89	A	C
ATOM	2250	CG	LYS	A	385	26.101	140.599	56.588	1.00175.33	A	C
ATOM	2251	CD	LYS	A	385	24.718	141.126	56.965	1.00177.89	A	C
ATOM	2252	CE	LYS	A	385	24.356	140.780	58.405	1.00179.02	A	C
ATOM	2253	NZ	LYS	A	385	22.974	141.214	58.760	1.00179.48	A	N
ATOM	2254	C	LYS	A	385	27.668	138.684	55.027	1.00 94.41	A	C
ATOM	2255	O	LYS	A	385	27.920	138.355	56.189	1.00 94.43	A	O
ATOM	2256	N	THR	A	386	27.376	137.802	54.076	1.00 75.18	A	N
ATOM	2257	CA	THR	A	386	27.308	136.379	54.362	1.00 76.30	A	C
ATOM	2258	CB	THR	A	386	25.865	135.838	54.118	1.00 51.08	A	C
ATOM	2259	OG1	THR	A	386	25.534	135.914	52.726	1.00 50.03	A	O
ATOM	2260	CG2	THR	A	386	24.854	136.667	54.911	1.00 50.94	A	C
ATOM	2261	C	THR	A	386	28.328	135.545	53.580	1.00 77.55	A	C
ATOM	2262	O	THR	A	386	28.983	134.673	54.153	1.00 77.88	A	O
ATOM	2263	N	LEU	A	387	28.472	135.808	52.284	1.00 46.03	A	N
ATOM	2264	CA	LEU	A	387	29.430	135.059	51.472	1.00 45.60	A	C
ATOM	2265	CB	LEU	A	387	29.108	135.168	49.990	1.00 28.96	A	C
ATOM	2266	CG	LEU	A	387	29.015	133.792	49.339	1.00 25.43	A	C
ATOM	2267	CD1	LEU	A	387	27.776	133.103	49.871	1.00 23.53	A	C
ATOM	2268	CD2	LEU	A	387	28.960	133.911	47.825	1.00 23.76	A	C
ATOM	2269	C	LEU	A	387	30.829	135.585	51.705	1.00 48.02	A	C
ATOM	2270	O	LEU	A	387	31.805	135.024	51.209	1.00 49.33	A	O
ATOM	2271	N	ARG	A	388	30.900	136.685	52.449	1.00 81.34	A	N
ATOM	2272	CA	ARG	A	388	32.151	137.336	52.813	1.00 83.08	A	C
ATOM	2273	CB	ARG	A	388	32.926	136.426	53.769	1.00148.48	A	C

ATOM	2274	CG	ARG	A	388	34.123	137.084	54.429	1.00149.70	A	C
ATOM	2275	CD	ARG	A	388	34.866	136.093	55.314	1.00151.22	A	C
ATOM	2276	NE	ARG	A	388	36.099	136.652	55.864	1.00154.03	A	N
ATOM	2277	CZ	ARG	A	388	36.940	135.980	56.644	1.00155.04	A	C
ATOM	2278	NH1	ARG	A	388	38.037	136.569	57.097	1.00155.61	A	N
ATOM	2279	NH2	ARG	A	388	36.684	134.719	56.973	1.00155.49	A	N
ATOM	2280	C	ARG	A	388	33.058	137.768	51.655	1.00 82.79	A	C
ATOM	2281	O	ARG	A	388	34.234	137.407	51.626	1.00 82.33	A	O
ATOM	2282	N	LEU	A	389	32.528	138.536	50.703	1.00 76.82	A	N
ATOM	2283	CA	LEU	A	389	33.356	139.015	49.592	1.00 78.14	A	C
ATOM	2284	CB	LEU	A	389	33.070	138.234	48.298	1.00 86.92	A	C
ATOM	2285	CG	LEU	A	389	31.669	137.915	47.774	1.00 87.95	A	C
ATOM	2286	CD1	LEU	A	389	30.840	139.172	47.565	1.00 87.29	A	C
ATOM	2287	CD2	LEU	A	389	31.833	137.162	46.463	1.00 88.60	A	C
ATOM	2288	C	LEU	A	389	33.217	140.517	49.352	1.00 78.91	A	C
ATOM	2289	O	LEU	A	389	32.129	141.077	49.461	1.00 77.45	A	O
ATOM	2290	N	ASN	A	390	34.337	141.167	49.045	1.00103.39	A	N
ATOM	2291	CA	ASN	A	390	34.353	142.605	48.804	1.00105.14	A	C
ATOM	2292	CB	ASN	A	390	35.770	143.157	48.989	1.00194.94	A	C
ATOM	2293	CG	ASN	A	390	36.050	143.581	50.421	1.00195.17	A	C
ATOM	2294	OD1	ASN	A	390	35.843	142.814	51.363	1.00195.16	A	O
ATOM	2295	ND2	ASN	A	390	36.527	144.810	50.589	1.00194.79	A	N
ATOM	2296	C	ASN	A	390	33.832	142.984	47.426	1.00106.37	A	C
ATOM	2297	O	ASN	A	390	33.197	142.179	46.748	1.00105.95	A	O
ATOM	2298	N	GLN	A	391	34.105	144.221	47.022	1.00203.67	A	N
ATOM	2299	CA	GLN	A	391	33.662	144.732	45.729	1.00203.67	A	C
ATOM	2300	CB	GLN	A	391	33.984	146.225	45.619	1.00157.13	A	C
ATOM	2301	CG	GLN	A	391	33.296	146.935	44.460	1.00158.68	A	C
ATOM	2302	CD	GLN	A	391	31.795	146.692	44.433	1.00159.60	A	C
ATOM	2303	OE1	GLN	A	391	31.141	146.642	45.477	1.00159.79	A	O
ATOM	2304	NE2	GLN	A	391	31.241	146.552	43.233	1.00160.01	A	N
ATOM	2305	C	GLN	A	391	34.312	143.976	44.575	1.00203.67	A	C
ATOM	2306	O	GLN	A	391	33.570	143.524	43.675	1.00203.67	A	O
ATOM	2307	OXT	GLN	A	391	35.556	143.854	44.581	1.00157.01	A	O
TER	2308		GLN	A	391					A	
ATOM	2309	CB	ALA	B	62	54.184	93.777	51.733	1.00 27.55	B	C
ATOM	2310	C	ALA	B	62	53.913	95.911	50.432	1.00 43.70	B	C
ATOM	2311	O	ALA	B	62	52.892	96.234	51.068	1.00 44.16	B	O
ATOM	2312	N	ALA	B	62	55.785	94.232	49.925	1.00 44.03	B	N
ATOM	2313	CA	ALA	B	62	54.369	94.429	50.372	1.00 43.69	B	C
ATOM	2314	N	LYS	B	63	54.669	96.792	49.763	1.00103.65	B	N
ATOM	2315	CA	LYS	B	63	54.394	98.241	49.725	1.00105.76	B	C
ATOM	2316	CB	LYS	B	63	54.979	98.915	50.975	1.00 62.62	B	C

ATOM	2317	CG	LYS	B	63	54.472	100.323	51.263	1.00	62.69	B C
ATOM	2318	CD	LYS	B	63	53.062	100.296	51.869	1.00	62.86	B C
ATOM	2319	CE	LYS	B	63	52.605	101.684	52.373	1.00	62.62	B C
ATOM	2320	NZ	LYS	B	63	51.314	101.684	53.160	1.00	62.56	B N
ATOM	2321	C	LYS	B	63	55.017	98.893	48.480	1.00	106.66	B C
ATOM	2322	O	LYS	B	63	55.296	100.089	48.482	1.00	106.43	B O
ATOM	2323	N	VAL	B	64	55.227	98.098	47.433	1.00	45.88	B N
ATOM	2324	CA	VAL	B	64	55.839	98.535	46.164	1.00	45.21	B C
ATOM	2325	CB	VAL	B	64	55.634	97.446	45.071	1.00	98.14	B C
ATOM	2326	CG1	VAL	B	64	56.335	96.151	45.479	1.00	98.12	B C
ATOM	2327	CG2	VAL	B	64	54.149	97.178	44.873	1.00	99.16	B C
ATOM	2328	C	VAL	B	64	55.385	99.899	45.604	1.00	45.77	B C
ATOM	2329	O	VAL	B	64	54.560	99.976	44.694	1.00	45.66	B O
ATOM	2330	N	GLY	B	65	55.961	100.975	46.123	1.00	63.83	B N
ATOM	2331	CA	GLY	B	65	55.570	102.303	45.683	1.00	63.37	B C
ATOM	2332	C	GLY	B	65	55.933	102.747	44.280	1.00	62.60	B C
ATOM	2333	O	GLY	B	65	56.893	103.499	44.114	1.00	62.29	B O
ATOM	2334	N	GLU	B	66	55.176	102.298	43.277	1.00	188.38	B N
ATOM	2335	CA	GLU	B	66	55.405	102.698	41.882	1.00	187.92	B C
ATOM	2336	CB	GLU	B	66	55.272	101.504	40.926	1.00	166.34	B C
ATOM	2337	CG	GLU	B	66	53.897	100.851	40.912	1.00	167.63	B C
ATOM	2338	CD	GLU	B	66	53.645	99.998	42.137	1.00	169.16	B C
ATOM	2339	OE1	GLU	B	66	54.283	98.930	42.259	1.00	169.98	B O
ATOM	2340	OE2	GLU	B	66	52.814	100.397	42.980	1.00	169.70	B O
ATOM	2341	C	GLU	B	66	54.349	103.749	41.534	1.00	187.56	B C
ATOM	2342	O	GLU	B	66	53.182	103.595	41.899	1.00	186.11	B O
ATOM	2343	N	LEU	B	67	54.743	104.807	40.827	1.00	78.81	B N
ATOM	2344	CA	LEU	B	67	53.792	105.868	40.496	1.00	77.41	B C
ATOM	2345	CB	LEU	B	67	53.351	106.566	41.790	1.00	133.93	B C
ATOM	2346	CG	LEU	B	67	54.350	107.483	42.522	1.00	131.87	B C
ATOM	2347	CD1	LEU	B	67	53.909	107.632	43.973	1.00	131.29	B C
ATOM	2348	CD2	LEU	B	67	55.763	106.914	42.474	1.00	129.01	B C
ATOM	2349	C	LEU	B	67	54.329	106.920	39.528	1.00	78.06	B C
ATOM	2350	O	LEU	B	67	55.373	106.732	38.899	1.00	77.64	B O
ATOM	2351	N	LYS	B	68	53.586	108.021	39.415	1.00	161.33	B N
ATOM	2352	CA	LYS	B	68	53.949	109.161	38.571	1.00	160.80	B C
ATOM	2353	CB	LYS	B	68	54.372	108.710	37.174	1.00	180.06	B C
ATOM	2354	CG	LYS	B	68	55.071	109.802	36.362	1.00	180.95	B C
ATOM	2355	CD	LYS	B	68	56.407	110.275	36.966	1.00	182.26	B C
ATOM	2356	CE	LYS	B	68	56.251	111.319	38.079	1.00	181.74	B C
ATOM	2357	NZ	LYS	B	68	56.115	110.734	39.445	1.00	180.37	B N
ATOM	2358	C	LYS	B	68	52.801	110.164	38.476	1.00	160.09	B C
ATOM	2359	O	LYS	B	68	51.918	110.166	39.333	1.00	159.78	B O

ATOM	2360	N	ASP	B	69	52.806	111.011	37.446	1.00162.59	B	N
ATOM	2361	CA	ASP	B	69	51.752	112.020	37.308	1.00162.10	B	C
ATOM	2362	CB	ASP	B	69	51.917	113.071	38.404	1.00160.80	B	C
ATOM	2363	CG	ASP	B	69	53.187	113.882	38.238	1.00161.36	B	C
ATOM	2364	OD1	ASP	B	69	53.219	114.758	37.348	1.00163.46	B	O
ATOM	2365	OD2	ASP	B	69	54.157	113.635	38.987	1.00160.60	B	O
ATOM	2366	C	ASP	B	69	51.665	112.741	35.960	1.00160.30	B	C
ATOM	2367	O	ASP	B	69	51.128	113.850	35.891	1.00159.72	B	O
ATOM	2368	N	ASP	B	70	52.184	112.124	34.901	1.00174.31	B	N
ATOM	2369	CA	ASP	B	70	52.147	112.724	33.566	1.00173.49	B	C
ATOM	2370	CB	ASP	B	70	52.604	114.184	33.606	1.00169.56	B	C
ATOM	2371	CG	ASP	B	70	54.102	114.333	33.370	1.00170.22	B	C
ATOM	2372	OD1	ASP	B	70	54.898	113.838	34.196	1.00169.30	B	O
ATOM	2373	OD2	ASP	B	70	54.483	114.943	32.350	1.00172.27	B	O
ATOM	2374	C	ASP	B	70	53.077	111.972	32.629	1.00172.32	B	C
ATOM	2375	O	ASP	B	70	53.120	112.248	31.430	1.00172.36	B	O
ATOM	2376	N	ASP	B	71	53.829	111.030	33.186	1.00107.55	B	N
ATOM	2377	CA	ASP	B	71	54.781	110.255	32.406	1.00106.46	B	C
ATOM	2378	CB	ASP	B	71	55.651	109.406	33.328	1.00152.56	B	C
ATOM	2379	CG	ASP	B	71	57.019	109.143	32.750	1.00151.39	B	C
ATOM	2380	OD1	ASP	B	71	57.103	108.863	31.536	1.00150.88	B	O
ATOM	2381	OD2	ASP	B	71	58.008	109.214	33.510	1.00150.94	B	O
ATOM	2382	C	ASP	B	71	54.080	109.351	31.405	1.00105.40	B	C
ATOM	2383	O	ASP	B	71	54.471	108.201	31.215	1.00104.14	B	O
ATOM	2384	N	PHE	B	72	53.043	109.876	30.765	1.00131.42	B	N
ATOM	2385	CA	PHE	B	72	52.299	109.107	29.783	1.00129.32	B	C
ATOM	2386	CB	PHE	B	72	50.882	108.837	30.283	1.00 69.93	B	C
ATOM	2387	CG	PHE	B	72	50.831	107.983	31.502	1.00 67.17	B	C
ATOM	2388	CD1	PHE	B	72	50.870	108.552	32.762	1.00 65.13	B	C
ATOM	2389	CD2	PHE	B	72	50.775	106.606	31.389	1.00 65.76	B	C
ATOM	2390	CE1	PHE	B	72	50.853	107.764	33.888	1.00 63.77	B	C
ATOM	2391	CE2	PHE	B	72	50.760	105.812	32.506	1.00 65.15	B	C
ATOM	2392	CZ	PHE	B	72	50.799	106.387	33.761	1.00 63.82	B	C
ATOM	2393	C	PHE	B	72	52.232	109.804	28.436	1.00129.56	B	C
ATOM	2394	O	PHE	B	72	52.594	110.972	28.308	1.00128.65	B	O
ATOM	2395	N	GLU	B	73	51.759	109.071	27.435	1.00 64.57	B	N
ATOM	2396	CA	GLU	B	73	51.632	109.591	26.082	1.00 65.93	B	C
ATOM	2397	CB	GLU	B	73	52.808	109.126	25.216	1.00109.43	B	C
ATOM	2398	CG	GLU	B	73	54.196	109.374	25.801	1.00111.28	B	C
ATOM	2399	CD	GLU	B	73	54.555	110.845	25.899	1.00112.82	B	C
ATOM	2400	OE1	GLU	B	73	55.726	111.149	26.215	1.00113.69	B	O
ATOM	2401	OE2	GLU	B	73	53.673	111.698	25.666	1.00115.23	B	O
ATOM	2402	C	GLU	B	73	50.337	109.071	25.474	1.00 67.40	B	C

ATOM	2403	O	GLU	B	73	50.234	107.890	25.153	1.00 67.27	B	O
ATOM	2404	N	ARG	B	74	49.352	109.949	25.323	1.00 86.41	B	N
ATOM	2405	CA	ARG	B	74	48.071	109.562	24.737	1.00 87.24	B	C
ATOM	2406	CB	ARG	B	74	47.191	110.804	24.539	1.00129.71	B	C
ATOM	2407	CG	ARG	B	74	47.192	111.771	25.726	1.00130.40	B	C
ATOM	2408	CD	ARG	B	74	46.643	113.146	25.339	1.00128.70	B	C
ATOM	2409	NE	ARG	B	74	47.276	114.229	26.096	1.00128.14	B	N
ATOM	2410	CZ	ARG	B	74	46.922	114.615	27.319	1.00127.75	B	C
ATOM	2411	NH1	ARG	B	74	45.921	114.014	27.950	1.00127.77	B	N
ATOM	2412	NH2	ARG	B	74	47.578	115.601	27.919	1.00127.52	B	N
ATOM	2413	C	ARG	B	74	48.378	108.914	23.384	1.00 87.57	B	C
ATOM	2414	O	ARG	B	74	49.265	109.376	22.662	1.00 87.06	B	O
ATOM	2415	N	ILE	B	75	47.669	107.841	23.043	1.00 89.30	B	N
ATOM	2416	CA	ILE	B	75	47.913	107.168	21.769	1.00 91.18	B	C
ATOM	2417	CB	ILE	B	75	49.030	106.115	21.882	1.00 77.93	B	C
ATOM	2418	CG2	ILE	B	75	50.290	106.749	22.448	1.00 79.59	B	C
ATOM	2419	CG1	ILE	B	75	48.553	104.939	22.736	1.00 78.15	B	C
ATOM	2420	CD1	ILE	B	75	49.575	103.830	22.865	1.00 78.88	B	C
ATOM	2421	C	ILE	B	75	46.699	106.463	21.175	1.00 91.33	B	C
ATOM	2422	O	ILE	B	75	46.765	105.967	20.052	1.00 90.67	B	O
ATOM	2423	N	SER	B	76	45.602	106.410	21.924	1.00128.82	B	N
ATOM	2424	CA	SER	B	76	44.374	105.758	21.465	1.00129.65	B	C
ATOM	2425	CB	SER	B	76	44.587	104.245	21.304	1.00203.67	B	C
ATOM	2426	OG	SER	B	76	45.477	103.935	20.245	1.00203.67	B	O
ATOM	2427	C	SER	B	76	43.263	105.991	22.481	1.00129.54	B	C
ATOM	2428	O	SER	B	76	43.147	105.245	23.450	1.00131.25	B	O
ATOM	2429	N	GLU	B	77	42.443	107.014	22.267	1.00 83.52	B	N
ATOM	2430	CA	GLU	B	77	41.369	107.288	23.212	1.00 82.23	B	C
ATOM	2431	CB	GLU	B	77	40.678	108.610	22.899	1.00179.96	B	C
ATOM	2432	CG	GLU	B	77	39.897	109.129	24.087	1.00178.72	B	C
ATOM	2433	CD	GLU	B	77	39.465	110.561	23.920	1.00178.13	B	C
ATOM	2434	OE1	GLU	B	77	40.324	111.396	23.559	1.00178.81	B	O
ATOM	2435	OE2	GLU	B	77	38.272	110.851	24.159	1.00176.44	B	O
ATOM	2436	C	GLU	B	77	40.362	106.146	23.227	1.00 82.94	B	C
ATOM	2437	O	GLU	B	77	39.962	105.638	22.180	1.00 83.42	B	O
ATOM	2438	N	LEU	B	78	39.949	105.754	24.425	1.00 60.08	B	N
ATOM	2439	CA	LEU	B	78	39.049	104.629	24.583	1.00 62.12	B	C
ATOM	2440	CB	LEU	B	78	39.441	103.849	25.841	1.00 96.73	B	C
ATOM	2441	CG	LEU	B	78	40.876	103.311	25.907	1.00 96.17	B	C
ATOM	2442	CD1	LEU	B	78	41.206	102.916	27.329	1.00 94.90	B	C
ATOM	2443	CD2	LEU	B	78	41.040	102.130	24.971	1.00 95.38	B	C
ATOM	2444	C	LEU	B	78	37.573	104.967	24.627	1.00 63.16	B	C
ATOM	2445	O	LEU	B	78	36.843	104.675	23.685	1.00 62.94	B	O

ATOM	2446	N	GLY	B	79	37.131	105.562	25.730	1.00	72.51	B	N
ATOM	2447	CA	GLY	B	79	35.728	105.910	25.874	1.00	74.33	B	C
ATOM	2448	C	GLY	B	79	35.473	106.862	27.029	1.00	75.27	B	C
ATOM	2449	O	GLY	B	79	36.407	107.280	27.726	1.00	76.05	B	O
ATOM	2450	N	ALA	B	80	34.203	107.210	27.229	1.00	84.31	B	N
ATOM	2451	CA	ALA	B	80	33.808	108.113	28.307	1.00	83.25	B	C
ATOM	2452	CB	ALA	B	80	34.016	109.559	27.885	1.00	95.52	B	C
ATOM	2453	C	ALA	B	80	32.351	107.888	28.682	1.00	84.07	B	C
ATOM	2454	O	ALA	B	80	31.668	107.054	28.084	1.00	84.77	B	O
ATOM	2455	N	GLY	B	81	31.883	108.636	29.677	1.00	110.56	B	N
ATOM	2456	CA	GLY	B	81	30.508	108.504	30.116	1.00	111.30	B	C
ATOM	2457	C	GLY	B	81	30.264	109.040	31.514	1.00	111.51	B	C
ATOM	2458	O	GLY	B	81	31.187	109.134	32.326	1.00	111.90	B	O
ATOM	2459	N	ASN	B	82	29.008	109.387	31.783	1.00	64.71	B	N
ATOM	2460	CA	ASN	B	82	28.564	109.922	33.068	1.00	66.76	B	C
ATOM	2461	CB	ASN	B	82	27.574	108.956	33.714	1.00	117.42	B	C
ATOM	2462	CG	ASN	B	82	26.139	109.355	33.477	1.00	118.87	B	C
ATOM	2463	OD1	ASN	B	82	25.706	110.428	33.892	1.00	119.08	B	O
ATOM	2464	ND2	ASN	B	82	25.390	108.492	32.806	1.00	119.79	B	N
ATOM	2465	C	ASN	B	82	29.616	110.294	34.108	1.00	67.24	B	C
ATOM	2466	O	ASN	B	82	29.603	109.758	35.212	1.00	67.92	B	O
ATOM	2467	N	GLY	B	83	30.514	111.215	33.768	1.00	123.47	B	N
ATOM	2468	CA	GLY	B	83	31.526	111.642	34.723	1.00	122.09	B	C
ATOM	2469	C	GLY	B	83	32.838	110.879	34.721	1.00	120.82	B	C
ATOM	2470	O	GLY	B	83	33.475	110.717	35.762	1.00	120.74	B	O
ATOM	2471	N	GLY	B	84	33.252	110.415	33.549	1.00	124.43	B	N
ATOM	2472	CA	GLY	B	84	34.495	109.681	33.451	1.00	121.64	B	C
ATOM	2473	C	GLY	B	84	34.872	109.425	32.007	1.00	120.47	B	C
ATOM	2474	O	GLY	B	84	34.071	108.899	31.231	1.00	120.84	B	O
ATOM	2475	N	VAL	B	85	36.089	109.810	31.640	1.00	93.27	B	N
ATOM	2476	CA	VAL	B	85	36.584	109.608	30.284	1.00	92.58	B	C
ATOM	2477	CB	VAL	B	85	36.729	110.943	29.536	1.00	51.56	B	C
ATOM	2478	CG1	VAL	B	85	37.385	111.992	30.435	1.00	52.10	B	C
ATOM	2479	CG2	VAL	B	85	37.545	110.727	28.281	1.00	51.94	B	C
ATOM	2480	C	VAL	B	85	37.938	108.904	30.332	1.00	90.91	B	C
ATOM	2481	O	VAL	B	85	38.872	109.381	30.982	1.00	89.70	B	O
ATOM	2482	N	VAL	B	86	38.037	107.765	29.648	1.00	68.49	B	N
ATOM	2483	CA	VAL	B	86	39.271	106.984	29.643	1.00	67.39	B	C
ATOM	2484	CB	VAL	B	86	39.050	105.563	30.200	1.00	69.07	B	C
ATOM	2485	CG1	VAL	B	86	38.085	105.607	31.367	1.00	69.99	B	C
ATOM	2486	CG2	VAL	B	86	38.534	104.657	29.114	1.00	69.83	B	C
ATOM	2487	C	VAL	B	86	39.858	106.853	28.252	1.00	65.82	B	C
ATOM	2488	O	VAL	B	86	39.190	107.104	27.250	1.00	65.54	B	O

ATOM	2489	N	THR	B	87	41.113	106.431	28.200	1.00	41.72	B	N
ATOM	2490	CA	THR	B	87	41.807	106.295	26.938	1.00	41.47	B	C
ATOM	2491	CB	THR	B	87	42.134	107.673	26.362	1.00	58.61	B	C
ATOM	2492	OG1	THR	B	87	43.188	107.545	25.397	1.00	59.45	B	O
ATOM	2493	CG2	THR	B	87	42.561	108.630	27.480	1.00	57.63	B	C
ATOM	2494	C	THR	B	87	43.113	105.535	27.058	1.00	41.69	B	C
ATOM	2495	O	THR	B	87	43.821	105.653	28.058	1.00	42.32	B	O
ATOM	2496	N	LYS	B	88	43.424	104.762	26.024	1.00	44.55	B	N
ATOM	2497	CA	LYS	B	88	44.662	103.997	25.971	1.00	44.37	B	C
ATOM	2498	CB	LYS	B	88	44.733	103.249	24.638	1.00	67.69	B	C
ATOM	2499	CG	LYS	B	88	45.948	102.371	24.444	1.00	69.52	B	C
ATOM	2500	CD	LYS	B	88	45.820	101.582	23.146	1.00	70.47	B	C
ATOM	2501	CE	LYS	B	88	46.991	100.625	22.956	1.00	71.83	B	C
ATOM	2502	NZ	LYS	B	88	46.878	99.798	21.720	1.00	71.95	B	N
ATOM	2503	C	LYS	B	88	45.807	105.009	26.092	1.00	45.17	B	C
ATOM	2504	O	LYS	B	88	45.792	106.039	25.419	1.00	42.89	B	O
ATOM	2505	N	VAL	B	89	46.785	104.737	26.954	1.00	83.47	B	N
ATOM	2506	CA	VAL	B	89	47.901	105.665	27.139	1.00	83.51	B	C
ATOM	2507	CB	VAL	B	89	47.489	106.855	28.038	1.00	174.05	B	C
ATOM	2508	CG1	VAL	B	89	47.100	106.360	29.420	1.00	175.70	B	C
ATOM	2509	CG2	VAL	B	89	48.624	107.856	28.125	1.00	173.50	B	C
ATOM	2510	C	VAL	B	89	49.127	104.995	27.746	1.00	83.77	B	C
ATOM	2511	O	VAL	B	89	49.082	104.503	28.873	1.00	83.32	B	O
ATOM	2512	N	GLN	B	90	50.227	105.005	26.994	1.00	99.42	B	N
ATOM	2513	CA	GLN	B	90	51.478	104.377	27.413	1.00	100.88	B	C
ATOM	2514	CB	GLN	B	90	52.357	104.104	26.193	1.00	81.42	B	C
ATOM	2515	CG	GLN	B	90	53.712	103.515	26.566	1.00	82.31	B	C
ATOM	2516	CD	GLN	B	90	54.536	103.116	25.361	1.00	83.55	B	C
ATOM	2517	OE1	GLN	B	90	55.594	102.499	25.491	1.00	85.84	B	O
ATOM	2518	NE2	GLN	B	90	54.055	103.466	24.179	1.00	84.40	B	N
ATOM	2519	C	GLN	B	90	52.332	105.101	28.453	1.00	101.73	B	C
ATOM	2520	O	GLN	B	90	52.444	106.327	28.442	1.00	102.44	B	O
ATOM	2521	N	HIS	B	91	52.942	104.312	29.339	1.00	112.50	B	N
ATOM	2522	CA	HIS	B	91	53.831	104.819	30.383	1.00	113.40	B	C
ATOM	2523	CB	HIS	B	91	53.743	103.962	31.644	1.00	83.66	B	C
ATOM	2524	CG	HIS	B	91	54.450	104.552	32.825	1.00	83.95	B	C
ATOM	2525	CD2	HIS	B	91	55.612	104.211	33.431	1.00	84.56	B	C
ATOM	2526	ND1	HIS	B	91	53.954	105.628	33.529	1.00	85.21	B	N
ATOM	2527	CE1	HIS	B	91	54.777	105.924	34.519	1.00	86.60	B	C
ATOM	2528	NE2	HIS	B	91	55.792	105.079	34.482	1.00	86.43	B	N
ATOM	2529	C	HIS	B	91	55.232	104.704	29.809	1.00	113.02	B	C
ATOM	2530	O	HIS	B	91	55.819	103.623	29.788	1.00	113.70	B	O
ATOM	2531	N	ARG	B	92	55.759	105.829	29.346	1.00	118.52	B	N

ATOM	2532	CA	ARG	B	92	57.075	105.882	28.727	1.00116.98	B	C
ATOM	2533	CB	ARG	B	92	57.542	107.340	28.652	1.00203.67	B	C
ATOM	2534	CG	ARG	B	92	58.871	107.519	27.945	1.00203.67	B	C
ATOM	2535	CD	ARG	B	92	59.295	108.977	27.903	1.00203.67	B	C
ATOM	2536	NE	ARG	B	92	60.553	109.148	27.182	1.00203.67	B	N
ATOM	2537	CZ	ARG	B	92	61.163	110.315	27.006	1.00203.67	B	C
ATOM	2538	NH1	ARG	B	92	62.305	110.375	26.334	1.00203.67	B	N
ATOM	2539	NH2	ARG	B	92	60.632	111.424	27.502	1.00203.67	B	N
ATOM	2540	C	ARG	B	92	58.178	105.017	29.345	1.00114.49	B	C
ATOM	2541	O	ARG	B	92	58.661	104.073	28.719	1.00114.59	B	O
ATOM	2542	N	PRO	B	93	58.582	105.320	30.587	1.00113.76	B	N
ATOM	2543	CD	PRO	B	93	57.909	106.238	31.519	1.00117.78	B	C
ATOM	2544	CA	PRO	B	93	59.636	104.578	31.283	1.00112.88	B	C
ATOM	2545	CB	PRO	B	93	59.524	105.085	32.718	1.00117.23	B	C
ATOM	2546	CG	PRO	B	93	58.978	106.467	32.548	1.00117.63	B	C
ATOM	2547	C	PRO	B	93	59.514	103.064	31.209	1.00110.58	B	C
ATOM	2548	O	PRO	B	93	60.518	102.358	31.172	1.00110.35	B	O
ATOM	2549	N	SER	B	94	58.285	102.568	31.184	1.00 71.16	B	N
ATOM	2550	CA	SER	B	94	58.051	101.132	31.146	1.00 70.27	B	C
ATOM	2551	CB	SER	B	94	57.014	100.764	32.204	1.00 62.16	B	C
ATOM	2552	OG	SER	B	94	55.824	101.508	32.014	1.00 62.79	B	O
ATOM	2553	C	SER	B	94	57.599	100.618	29.784	1.00 69.55	B	C
ATOM	2554	O	SER	B	94	57.612	99.410	29.531	1.00 69.77	B	O
ATOM	2555	N	GLY	B	95	57.209	101.527	28.900	1.00 66.99	B	N
ATOM	2556	CA	GLY	B	95	56.753	101.095	27.595	1.00 66.18	B	C
ATOM	2557	C	GLY	B	95	55.664	100.076	27.829	1.00 66.47	B	C
ATOM	2558	O	GLY	B	95	55.886	98.877	27.674	1.00 67.36	B	O
ATOM	2559	N	LEU	B	96	54.494	100.571	28.228	1.00 92.99	B	N
ATOM	2560	CA	LEU	B	96	53.321	99.748	28.526	1.00 91.16	B	C
ATOM	2561	CB	LEU	B	96	53.336	99.325	29.998	1.00 48.20	B	C
ATOM	2562	CG	LEU	B	96	54.028	98.027	30.396	1.00 46.86	B	C
ATOM	2563	CD1	LEU	B	96	54.253	98.024	31.887	1.00 47.31	B	C
ATOM	2564	CD2	LEU	B	96	53.175	96.838	29.961	1.00 46.32	B	C
ATOM	2565	C	LEU	B	96	52.019	100.498	28.255	1.00 89.93	B	C
ATOM	2566	O	LEU	B	96	51.730	101.504	28.902	1.00 89.41	B	O
ATOM	2567	N	ILE	B	97	51.231	100.010	27.305	1.00 70.75	B	N
ATOM	2568	CA	ILE	B	97	49.964	100.658	27.011	1.00 71.51	B	C
ATOM	2569	CB	ILE	B	97	49.347	100.126	25.711	1.00 61.48	B	C
ATOM	2570	CG2	ILE	B	97	50.315	100.331	24.576	1.00 60.88	B	C
ATOM	2571	CG1	ILE	B	97	49.040	98.634	25.837	1.00 63.49	B	C
ATOM	2572	CD1	ILE	B	97	48.361	98.039	24.616	1.00 64.69	B	C
ATOM	2573	C	ILE	B	97	49.011	100.378	28.167	1.00 71.13	B	C
ATOM	2574	O	ILE	B	97	48.606	99.238	28.389	1.00 71.05	B	O

ATOM	2575	N	MET	B	98	48.664	101.419	28.912	1.00	62.24	B	N
ATOM	2576	CA	MET	B	98	47.769	101.258	30.042	1.00	62.91	B	C
ATOM	2577	CB	MET	B	98	48.182	102.196	31.161	1.00	40.92	B	C
ATOM	2578	CG	MET	B	98	49.644	102.488	31.156	1.00	42.91	B	C
ATOM	2579	SD	MET	B	98	50.472	101.914	32.614	1.00	41.69	B	S
ATOM	2580	CE	MET	B	98	49.900	103.110	33.800	1.00	42.58	B	C
ATOM	2581	C	MET	B	98	46.343	101.574	29.635	1.00	62.95	B	C
ATOM	2582	O	MET	B	98	45.755	100.927	28.764	1.00	62.68	B	O
ATOM	2583	N	ALA	B	99	45.800	102.590	30.284	1.00	53.35	B	N
ATOM	2584	CA	ALA	B	99	44.449	103.043	30.043	1.00	51.50	B	C
ATOM	2585	CB	ALA	B	99	43.485	101.881	30.109	1.00	74.31	B	C
ATOM	2586	C	ALA	B	99	44.204	103.997	31.183	1.00	49.86	B	C
ATOM	2587	O	ALA	B	99	43.971	103.574	32.313	1.00	48.99	B	O
ATOM	2588	N	ARG	B	100	44.289	105.288	30.892	1.00	62.75	B	N
ATOM	2589	CA	ARG	B	100	44.089	106.307	31.911	1.00	62.64	B	C
ATOM	2590	CB	ARG	B	100	44.862	107.576	31.529	1.00	70.50	B	C
ATOM	2591	CG	ARG	B	100	45.000	108.632	32.614	1.00	69.16	B	C
ATOM	2592	CD	ARG	B	100	45.536	109.897	31.984	1.00	69.70	B	C
ATOM	2593	NE	ARG	B	100	45.969	110.897	32.952	1.00	70.32	B	N
ATOM	2594	CZ	ARG	B	100	47.037	110.777	33.737	1.00	70.23	B	C
ATOM	2595	NH1	ARG	B	100	47.789	109.689	33.677	1.00	69.31	B	N
ATOM	2596	NH2	ARG	B	100	47.367	111.759	34.567	1.00	69.09	B	N
ATOM	2597	C	ARG	B	100	42.607	106.620	32.040	1.00	63.22	B	C
ATOM	2598	O	ARG	B	100	41.899	106.760	31.042	1.00	60.21	B	O
ATOM	2599	N	LYS	B	101	42.132	106.705	33.276	1.00	46.13	B	N
ATOM	2600	CA	LYS	B	101	40.738	107.028	33.495	1.00	46.76	B	C
ATOM	2601	CB	LYS	B	101	40.057	106.042	34.437	1.00	63.93	B	C
ATOM	2602	CG	LYS	B	101	38.590	106.381	34.599	1.00	64.09	B	C
ATOM	2603	CD	LYS	B	101	37.815	105.331	35.339	1.00	63.46	B	C
ATOM	2604	CE	LYS	B	101	36.335	105.607	35.211	1.00	63.34	B	C
ATOM	2605	NZ	LYS	B	101	35.536	104.646	35.986	1.00	63.22	B	N
ATOM	2606	C	LYS	B	101	40.653	108.406	34.093	1.00	48.12	B	C
ATOM	2607	O	LYS	B	101	41.081	108.638	35.224	1.00	46.53	B	O
ATOM	2608	N	LEU	B	102	40.098	109.325	33.318	1.00	71.93	B	N
ATOM	2609	CA	LEU	B	102	39.948	110.688	33.769	1.00	74.86	B	C
ATOM	2610	CB	LEU	B	102	40.131	111.647	32.595	1.00	103.17	B	C
ATOM	2611	CG	LEU	B	102	41.456	111.580	31.834	1.00	104.53	B	C
ATOM	2612	CD1	LEU	B	102	41.435	112.598	30.698	1.00	103.10	B	C
ATOM	2613	CD2	LEU	B	102	42.605	111.861	32.780	1.00	105.27	B	C
ATOM	2614	C	LEU	B	102	38.582	110.910	34.407	1.00	76.67	B	C
ATOM	2615	O	LEU	B	102	37.581	111.103	33.717	1.00	77.47	B	O
ATOM	2616	N	ILE	B	103	38.546	110.840	35.731	1.00	74.86	B	N
ATOM	2617	CA	ILE	B	103	37.323	111.091	36.478	1.00	76.22	B	C

ATOM	2618	CB	ILE	B	103	37.187	110.169	37.691	1.00	82.83	B	C
ATOM	2619	CG2	ILE	B	103	35.887	110.456	38.417	1.00	81.02	B	C
ATOM	2620	CG1	ILE	B	103	37.246	108.714	37.243	1.00	84.40	B	C
ATOM	2621	CD1	ILE	B	103	37.110	107.732	38.379	1.00	83.96	B	C
ATOM	2622	C	ILE	B	103	37.613	112.483	36.987	1.00	78.81	B	C
ATOM	2623	O	ILE	B	103	38.054	112.648	38.122	1.00	80.04	B	O
ATOM	2624	N	HIS	B	104	37.403	113.486	36.143	1.00	135.10	B	N
ATOM	2625	CA	HIS	B	104	37.698	114.842	36.562	1.00	136.46	B	C
ATOM	2626	CB	HIS	B	104	37.261	115.867	35.529	1.00	119.66	B	C
ATOM	2627	CG	HIS	B	104	37.692	117.254	35.879	1.00	119.49	B	C
ATOM	2628	CD2	HIS	B	104	37.003	118.300	36.392	1.00	120.42	B	C
ATOM	2629	ND1	HIS	B	104	39.009	117.656	35.816	1.00	119.25	B	N
ATOM	2630	CE1	HIS	B	104	39.113	118.888	36.277	1.00	120.16	B	C
ATOM	2631	NE2	HIS	B	104	37.910	119.302	36.634	1.00	120.74	B	N
ATOM	2632	C	HIS	B	104	37.028	115.179	37.874	1.00	137.73	B	C
ATOM	2633	O	HIS	B	104	37.547	114.864	38.944	1.00	137.55	B	O
ATOM	2634	N	LEU	B	105	35.876	115.832	37.790	1.00	117.96	B	N
ATOM	2635	CA	LEU	B	105	35.149	116.196	38.990	1.00	118.37	B	C
ATOM	2636	CB	LEU	B	105	34.593	114.938	39.648	1.00	128.33	B	C
ATOM	2637	CG	LEU	B	105	34.103	115.090	41.082	1.00	130.30	B	C
ATOM	2638	CD1	LEU	B	105	32.977	116.110	41.151	1.00	130.71	B	C
ATOM	2639	CD2	LEU	B	105	33.648	113.740	41.577	1.00	129.96	B	C
ATOM	2640	C	LEU	B	105	36.092	116.890	39.953	1.00	120.03	B	C
ATOM	2641	O	LEU	B	105	36.685	116.239	40.810	1.00	117.59	B	O
ATOM	2642	N	GLU	B	106	36.236	118.204	39.807	1.00	134.20	B	N
ATOM	2643	CA	GLU	B	106	37.120	118.971	40.680	1.00	136.57	B	C
ATOM	2644	CB	GLU	B	106	36.711	120.445	40.693	1.00	203.67	B	C
ATOM	2645	CG	GLU	B	106	37.293	121.254	41.855	1.00	203.67	B	C
ATOM	2646	CD	GLU	B	106	38.810	121.173	41.956	1.00	203.67	B	C
ATOM	2647	OE1	GLU	B	106	39.338	120.091	42.291	1.00	203.67	B	O
ATOM	2648	OE2	GLU	B	106	39.479	122.197	41.702	1.00	203.67	B	O
ATOM	2649	C	GLU	B	106	37.139	118.433	42.110	1.00	137.32	B	C
ATOM	2650	O	GLU	B	106	36.216	118.674	42.896	1.00	137.01	B	O
ATOM	2651	N	ILE	B	107	38.203	117.701	42.431	1.00	181.30	B	N
ATOM	2652	CA	ILE	B	107	38.376	117.112	43.753	1.00	182.71	B	C
ATOM	2653	CB	ILE	B	107	39.208	115.812	43.685	1.00	134.90	B	C
ATOM	2654	CG2	ILE	B	107	39.263	115.164	45.055	1.00	133.68	B	C
ATOM	2655	CG1	ILE	B	107	38.594	114.841	42.676	1.00	137.21	B	C
ATOM	2656	CD1	ILE	B	107	37.202	114.378	43.038	1.00	138.69	B	C
ATOM	2657	C	ILE	B	107	39.106	118.080	44.673	1.00	182.77	B	C
ATOM	2658	O	ILE	B	107	40.295	118.343	44.490	1.00	182.17	B	O
ATOM	2659	N	LYS	B	108	38.395	118.613	45.660	1.00	148.35	B	N
ATOM	2660	CA	LYS	B	108	39.007	119.537	46.602	1.00	149.22	B	C

ATOM	2661	CB	LYS	B	108	38.020	119.878	47.724	1.00132.63	B	C
ATOM	2662	CG	LYS	B	108	37.018	118.778	48.040	1.00133.81	B	C
ATOM	2663	CD	LYS	B	108	36.054	119.220	49.132	1.00135.07	B	C
ATOM	2664	CE	LYS	B	108	34.929	118.214	49.329	1.00136.17	B	C
ATOM	2665	NZ	LYS	B	108	34.067	118.087	48.119	1.00136.87	B	N
ATOM	2666	C	LYS	B	108	40.276	118.914	47.177	1.00147.96	B	C
ATOM	2667	O	LYS	B	108	40.297	117.732	47.518	1.00148.89	B	O
ATOM	2668	N	PRO	B	109	41.360	119.703	47.275	1.00110.67	B	N
ATOM	2669	CD	PRO	B	109	41.464	121.122	46.892	1.00154.46	B	C
ATOM	2670	CA	PRO	B	109	42.636	119.217	47.810	1.00110.42	B	C
ATOM	2671	CB	PRO	B	109	43.472	120.489	47.905	1.00153.65	B	C
ATOM	2672	CG	PRO	B	109	42.959	121.308	46.763	1.00153.35	B	C
ATOM	2673	C	PRO	B	109	42.440	118.559	49.165	1.00108.86	B	C
ATOM	2674	O	PRO	B	109	43.192	117.668	49.553	1.00109.28	B	O
ATOM	2675	N	ALA	B	110	41.411	119.012	49.871	1.00151.90	B	N
ATOM	2676	CA	ALA	B	110	41.077	118.502	51.192	1.00152.25	B	C
ATOM	2677	CB	ALA	B	110	39.809	119.185	51.703	1.00136.51	B	C
ATOM	2678	C	ALA	B	110	40.892	116.990	51.216	1.00150.32	B	C
ATOM	2679	O	ALA	B	110	41.471	116.303	52.058	1.00149.09	B	O
ATOM	2680	N	ILE	B	111	40.094	116.473	50.286	1.00 97.29	B	N
ATOM	2681	CA	ILE	B	111	39.817	115.043	50.247	1.00 96.55	B	C
ATOM	2682	CB	ILE	B	111	38.355	114.769	49.834	1.00 43.90	B	C
ATOM	2683	CG2	ILE	B	111	37.417	115.601	50.681	1.00 44.43	B	C
ATOM	2684	CG1	ILE	B	111	38.160	115.091	48.354	1.00 45.18	B	C
ATOM	2685	CD1	ILE	B	111	36.747	114.841	47.841	1.00 46.60	B	C
ATOM	2686	C	ILE	B	111	40.713	114.166	49.376	1.00 94.53	B	C
ATOM	2687	O	ILE	B	111	41.065	113.067	49.785	1.00 92.61	B	O
ATOM	2688	N	ARG	B	112	41.082	114.626	48.185	1.00 72.07	B	N
ATOM	2689	CA	ARG	B	112	41.914	113.802	47.319	1.00 73.43	B	C
ATOM	2690	CB	ARG	B	112	42.405	114.591	46.102	1.00110.65	B	C
ATOM	2691	CG	ARG	B	112	42.702	116.062	46.328	1.00111.16	B	C
ATOM	2692	CD	ARG	B	112	43.255	116.670	45.042	1.00111.86	B	C
ATOM	2693	NE	ARG	B	112	42.410	116.375	43.886	1.00114.17	B	N
ATOM	2694	CZ	ARG	B	112	42.794	116.518	42.623	1.00115.48	B	C
ATOM	2695	NH1	ARG	B	112	44.015	116.952	42.347	1.00115.70	B	N
ATOM	2696	NH2	ARG	B	112	41.960	116.227	41.635	1.00116.18	B	N
ATOM	2697	C	ARG	B	112	43.089	113.146	48.025	1.00 73.13	B	C
ATOM	2698	O	ARG	B	112	43.457	112.027	47.675	1.00 73.06	B	O
ATOM	2699	N	ASN	B	113	43.678	113.822	49.013	1.00180.29	B	N
ATOM	2700	CA	ASN	B	113	44.800	113.243	49.765	1.00181.45	B	C
ATOM	2701	CB	ASN	B	113	45.309	114.211	50.849	1.00120.28	B	C
ATOM	2702	CG	ASN	B	113	45.979	115.452	50.277	1.00120.20	B	C
ATOM	2703	OD1	ASN	B	113	45.427	116.550	50.330	1.00120.34	B	O

ATOM	2704	ND2	ASN	B	113	47.177	115.280	49.732	1.00119.84	B	N
ATOM	2705	C	ASN	B	113	44.278	111.973	50.438	1.00182.09	B	C
ATOM	2706	O	ASN	B	113	45.019	111.015	50.678	1.00181.84	B	O
ATOM	2707	N	GLN	B	114	42.983	112.000	50.739	1.00124.93	B	N
ATOM	2708	CA	GLN	B	114	42.266	110.904	51.372	1.00125.15	B	C
ATOM	2709	CB	GLN	B	114	41.177	111.480	52.283	1.00145.34	B	C
ATOM	2710	CG	GLN	B	114	40.124	110.498	52.758	1.00149.06	B	C
ATOM	2711	CD	GLN	B	114	40.708	109.304	53.472	1.00152.35	B	C
ATOM	2712	OE1	GLN	B	114	41.229	108.389	52.841	1.00153.33	B	O
ATOM	2713	NE2	GLN	B	114	40.634	109.308	54.798	1.00154.08	B	N
ATOM	2714	C	GLN	B	114	41.655	110.018	50.288	1.00123.25	B	C
ATOM	2715	O	GLN	B	114	41.624	108.797	50.417	1.00121.59	B	O
ATOM	2716	N	ILE	B	115	41.174	110.641	49.216	1.00 78.11	B	N
ATOM	2717	CA	ILE	B	115	40.590	109.899	48.102	1.00 74.64	B	C
ATOM	2718	CB	ILE	B	115	40.119	110.837	46.969	1.00 97.49	B	C
ATOM	2719	CG2	ILE	B	115	40.009	110.061	45.656	1.00 96.43	B	C
ATOM	2720	CG1	ILE	B	115	38.786	111.481	47.357	1.00 97.60	B	C
ATOM	2721	CD1	ILE	B	115	38.162	112.289	46.255	1.00 99.10	B	C
ATOM	2722	C	ILE	B	115	41.646	108.962	47.551	1.00 74.63	B	C
ATOM	2723	O	ILE	B	115	41.344	107.897	47.020	1.00 73.93	B	O
ATOM	2724	N	ILE	B	116	42.897	109.376	47.676	1.00 69.86	B	N
ATOM	2725	CA	ILE	B	116	43.996	108.552	47.222	1.00 68.92	B	C
ATOM	2726	CB	ILE	B	116	45.267	109.390	47.015	1.00128.18	B	C
ATOM	2727	CG2	ILE	B	116	46.477	108.482	46.841	1.00128.11	B	C
ATOM	2728	CG1	ILE	B	116	45.083	110.288	45.792	1.00129.68	B	C
ATOM	2729	CD1	ILE	B	116	44.708	109.528	44.535	1.00131.72	B	C
ATOM	2730	C	ILE	B	116	44.236	107.494	48.295	1.00 69.57	B	C
ATOM	2731	O	ILE	B	116	44.692	106.388	48.010	1.00 69.62	B	O
ATOM	2732	N	ARG	B	117	43.909	107.840	49.533	1.00101.63	B	N
ATOM	2733	CA	ARG	B	117	44.084	106.908	50.630	1.00100.58	B	C
ATOM	2734	CB	ARG	B	117	43.872	107.615	51.975	1.00162.45	B	C
ATOM	2735	CG	ARG	B	117	44.123	106.728	53.201	1.00164.91	B	C
ATOM	2736	CD	ARG	B	117	43.137	107.002	54.347	1.00169.29	B	C
ATOM	2737	NE	ARG	B	117	43.530	108.083	55.254	1.00173.29	B	N
ATOM	2738	CZ	ARG	B	117	43.670	109.362	54.913	1.00174.87	B	C
ATOM	2739	NH1	ARG	B	117	43.457	109.755	53.668	1.00174.71	B	N
ATOM	2740	NH2	ARG	B	117	44.015	110.257	55.828	1.00175.95	B	N
ATOM	2741	C	ARG	B	117	43.090	105.752	50.491	1.00 99.31	B	C
ATOM	2742	O	ARG	B	117	43.356	104.639	50.960	1.00 99.97	B	O
ATOM	2743	N	GLU	B	118	41.955	106.007	49.839	1.00120.49	B	N
ATOM	2744	CA	GLU	B	118	40.927	104.977	49.671	1.00118.64	B	C
ATOM	2745	CB	GLU	B	118	39.530	105.601	49.756	1.00 63.52	B	C
ATOM	2746	CG	GLU	B	118	39.263	106.306	51.076	1.00 64.28	B	C

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ATOM   2747  CD  GLU B 118     37.804 106.674  51.265  1.00 65.00      B    C
ATOM   2748  OE1 GLU B 118     37.223 107.285  50.343  1.00 64.31      B    O
ATOM   2749  OE2 GLU B 118     37.239 106.359  52.338  1.00 64.91      B    O
ATOM   2750  C   GLU B 118     41.048 104.168  48.385  1.00116.21      B    C
ATOM   2751  O   GLU B 118     40.684 102.994  48.352  1.00115.57      B    O
ATOM   2752  N   LEU B 119     41.560 104.793  47.331  1.00 79.58      B    N
ATOM   2753  CA  LEU B 119     41.729 104.114  46.048  1.00 75.76      B    C
ATOM   2754  CB  LEU B 119     41.753 105.141  44.912  1.00 35.82      B    C
ATOM   2755  CG  LEU B 119     40.374 105.455  44.337  1.00 34.53      B    C
ATOM   2756  CD1 LEU B 119     40.441 106.440  43.189  1.00 35.16      B    C
ATOM   2757  CD2 LEU B 119     39.818 104.187  43.845  1.00 35.33      B    C
ATOM   2758  C   LEU B 119     42.993 103.256  45.987  1.00 75.81      B    C
ATOM   2759  O   LEU B 119     43.288 102.628  44.966  1.00 76.48      B    O
ATOM   2760  N   GLN B 120     43.725 103.218  47.094  1.00 79.60      B    N
ATOM   2761  CA  GLN B 120     44.966 102.465  47.164  1.00 79.88      B    C
ATOM   2762  CB  GLN B 120     45.911 103.137  48.163  1.00 64.89      B    C
ATOM   2763  CG  GLN B 120     46.525 104.438  47.650  1.00 66.53      B    C
ATOM   2764  CD  GLN B 120     47.378 104.220  46.425  1.00 67.61      B    C
ATOM   2765  OE1 GLN B 120     48.290 103.401  46.438  1.00 67.75      B    O
ATOM   2766  NE2 GLN B 120     47.087 104.952  45.359  1.00 66.91      B    N
ATOM   2767  C   GLN B 120     44.831 100.977  47.486  1.00 77.86      B    C
ATOM   2768  O   GLN B 120     45.811 100.236  47.411  1.00 76.48      B    O
ATOM   2769  N   VAL B 121     43.634 100.534  47.852  1.00 33.28      B    N
ATOM   2770  CA  VAL B 121     43.431  99.119  48.145  1.00 32.65      B    C
ATOM   2771  CB  VAL B 121     42.118  98.851  48.929  1.00 32.30      B    C
ATOM   2772  CG1 VAL B 121     41.781 100.046  49.808  1.00 34.40      B    C
ATOM   2773  CG2 VAL B 121     40.980  98.521  47.966  1.00 34.65      B    C
ATOM   2774  C   VAL B 121     43.341  98.405  46.808  1.00 30.01      B    C
ATOM   2775  O   VAL B 121     43.442  97.188  46.739  1.00 27.78      B    O
ATOM   2776  N   LEU B 122     43.128  99.178  45.748  1.00 43.35      B    N
ATOM   2777  CA  LEU B 122     43.051  98.634  44.405  1.00 41.12      B    C
ATOM   2778  CB  LEU B 122     42.891  99.765  43.403  1.00 49.66      B    C
ATOM   2779  CG  LEU B 122     41.458 100.018  42.946  1.00 49.64      B    C
ATOM   2780  CD1 LEU B 122     41.245 101.520  42.794  1.00 48.51      B    C
ATOM   2781  CD2 LEU B 122     41.181  99.245  41.631  1.00 48.83      B    C
ATOM   2782  C   LEU B 122     44.381  97.944  44.201  1.00 38.18      B    C
ATOM   2783  O   LEU B 122     44.500  96.959  43.462  1.00 36.97      B    O
ATOM   2784  N   HIS B 123     45.377  98.498  44.886  1.00 55.34      B    N
ATOM   2785  CA  HIS B 123     46.741  97.998  44.880  1.00 56.02      B    C
ATOM   2786  CB  HIS B 123     47.638  98.999  45.615  1.00 42.65      B    C
ATOM   2787  CG  HIS B 123     48.357  99.952  44.708  1.00 40.05      B    C
ATOM   2788  CD2 HIS B 123     48.804  99.809  43.437  1.00 39.45      B    C
ATOM   2789  ND1 HIS B 123     48.746 101.212  45.110  1.00 40.22      B    N
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ATOM	2790	CE1	HIS	B	123	49.401	101.804	44.126	1.00	40.47	B	C
ATOM	2791	NE2	HIS	B	123	49.451	100.975	43.101	1.00	39.93	B	N
ATOM	2792	C	HIS	B	123	46.738	96.644	45.595	1.00	58.19	B	C
ATOM	2793	O	HIS	B	123	47.427	95.700	45.189	1.00	57.41	B	O
ATOM	2794	N	GLU	B	124	45.948	96.556	46.658	1.00	41.93	B	N
ATOM	2795	CA	GLU	B	124	45.832	95.329	47.414	1.00	43.66	B	C
ATOM	2796	CB	GLU	B	124	45.421	95.665	48.843	1.00	73.24	B	C
ATOM	2797	CG	GLU	B	124	46.531	96.349	49.629	1.00	79.05	B	C
ATOM	2798	CD	GLU	B	124	46.019	97.292	50.721	1.00	83.21	B	C
ATOM	2799	OE1	GLU	B	124	45.635	98.444	50.398	1.00	86.27	B	O
ATOM	2800	OE2	GLU	B	124	45.998	96.879	51.904	1.00	84.56	B	O
ATOM	2801	C	GLU	B	124	44.836	94.346	46.765	1.00	45.79	B	C
ATOM	2802	O	GLU	B	124	44.490	93.333	47.363	1.00	47.68	B	O
ATOM	2803	N	CYS	B	125	44.390	94.634	45.541	1.00	62.70	B	N
ATOM	2804	CA	CYS	B	125	43.446	93.756	44.838	1.00	63.02	B	C
ATOM	2805	CB	CYS	B	125	42.267	94.537	44.272	1.00	28.50	B	C
ATOM	2806	SG	CYS	B	125	41.248	95.405	45.422	1.00	31.06	B	S
ATOM	2807	C	CYS	B	125	44.101	93.070	43.660	1.00	61.11	B	C
ATOM	2808	O	CYS	B	125	44.792	93.712	42.872	1.00	62.16	B	O
ATOM	2809	N	ASN	B	126	43.859	91.772	43.518	1.00	40.37	B	N
ATOM	2810	CA	ASN	B	126	44.419	91.022	42.402	1.00	42.14	B	C
ATOM	2811	CB	ASN	B	126	45.948	90.889	42.536	1.00	77.47	B	C
ATOM	2812	CG	ASN	B	126	46.389	89.492	42.961	1.00	79.44	B	C
ATOM	2813	OD1	ASN	B	126	46.378	89.153	44.149	1.00	78.88	B	O
ATOM	2814	ND2	ASN	B	126	46.772	88.671	41.986	1.00	79.32	B	N
ATOM	2815	C	ASN	B	126	43.790	89.645	42.248	1.00	41.30	B	C
ATOM	2816	O	ASN	B	126	43.878	88.794	43.123	1.00	42.02	B	O
ATOM	2817	N	SER	B	127	43.138	89.453	41.114	1.00	30.58	B	N
ATOM	2818	CA	SER	B	127	42.495	88.203	40.767	1.00	28.08	B	C
ATOM	2819	CB	SER	B	127	41.094	88.129	41.343	1.00	25.30	B	C
ATOM	2820	OG	SER	B	127	40.347	87.137	40.666	1.00	25.67	B	O
ATOM	2821	C	SER	B	127	42.392	88.226	39.271	1.00	28.31	B	C
ATOM	2822	O	SER	B	127	42.253	89.291	38.678	1.00	31.17	B	O
ATOM	2823	N	PRO	B	128	42.473	87.063	38.629	1.00	17.20	B	N
ATOM	2824	CD	PRO	B	128	43.059	85.805	39.110	1.00	51.72	B	C
ATOM	2825	CA	PRO	B	128	42.372	87.056	37.170	1.00	17.50	B	C
ATOM	2826	CB	PRO	B	128	42.663	85.603	36.826	1.00	52.25	B	C
ATOM	2827	CG	PRO	B	128	43.680	85.246	37.850	1.00	51.10	B	C
ATOM	2828	C	PRO	B	128	41.011	87.521	36.670	1.00	15.86	B	C
ATOM	2829	O	PRO	B	128	40.660	87.322	35.510	1.00	16.85	B	O
ATOM	2830	N	TYR	B	129	40.263	88.153	37.564	1.00	29.83	B	N
ATOM	2831	CA	TYR	B	129	38.930	88.649	37.263	1.00	28.69	B	C
ATOM	2832	CB	TYR	B	129	37.901	87.827	38.011	1.00	40.87	B	C

ATOM	2833	CG	TYR	B	129	38.090	86.362	37.794	1.00	41.05	B	C
ATOM	2834	CD1	TYR	B	129	37.872	85.798	36.545	1.00	43.05	B	C
ATOM	2835	CE1	TYR	B	129	38.008	84.454	36.350	1.00	44.11	B	C
ATOM	2836	CD2	TYR	B	129	38.459	85.537	38.836	1.00	40.80	B	C
ATOM	2837	CE2	TYR	B	129	38.599	84.199	38.648	1.00	41.60	B	C
ATOM	2838	CZ	TYR	B	129	38.367	83.657	37.404	1.00	42.60	B	C
ATOM	2839	OH	TYR	B	129	38.453	82.302	37.220	1.00	42.62	B	O
ATOM	2840	C	TYR	B	129	38.748	90.104	37.621	1.00	28.88	B	C
ATOM	2841	O	TYR	B	129	37.683	90.664	37.397	1.00	30.58	B	O
ATOM	2842	N	ILE	B	130	39.764	90.704	38.222	1.00	54.75	B	N
ATOM	2843	CA	ILE	B	130	39.683	92.109	38.552	1.00	54.92	B	C
ATOM	2844	CB	ILE	B	130	39.932	92.371	40.039	1.00	50.09	B	C
ATOM	2845	CG2	ILE	B	130	40.163	93.863	40.274	1.00	51.36	B	C
ATOM	2846	CG1	ILE	B	130	38.713	91.926	40.851	1.00	50.06	B	C
ATOM	2847	CD1	ILE	B	130	38.279	90.507	40.606	1.00	54.25	B	C
ATOM	2848	C	ILE	B	130	40.740	92.780	37.694	1.00	53.13	B	C
ATOM	2849	O	ILE	B	130	41.839	92.250	37.525	1.00	51.93	B	O
ATOM	2850	N	VAL	B	131	40.387	93.931	37.133	1.00	27.94	B	N
ATOM	2851	CA	VAL	B	131	41.264	94.673	36.250	1.00	27.83	B	C
ATOM	2852	CB	VAL	B	131	40.498	95.843	35.643	1.00	18.06	B	C
ATOM	2853	CG1	VAL	B	131	41.436	97.010	35.379	1.00	17.46	B	C
ATOM	2854	CG2	VAL	B	131	39.829	95.372	34.356	1.00	16.90	B	C
ATOM	2855	C	VAL	B	131	42.552	95.170	36.882	1.00	29.77	B	C
ATOM	2856	O	VAL	B	131	42.526	95.875	37.881	1.00	28.59	B	O
ATOM	2857	N	GLY	B	132	43.678	94.781	36.288	1.00	36.19	B	N
ATOM	2858	CA	GLY	B	132	44.972	95.197	36.793	1.00	41.18	B	C
ATOM	2859	C	GLY	B	132	44.942	96.679	37.079	1.00	45.29	B	C
ATOM	2860	O	GLY	B	132	44.387	97.443	36.292	1.00	47.11	B	O
ATOM	2861	N	PHE	B	133	45.539	97.088	38.195	1.00	39.71	B	N
ATOM	2862	CA	PHE	B	133	45.544	98.494	38.586	1.00	41.43	B	C
ATOM	2863	CB	PHE	B	133	44.718	98.670	39.868	1.00	54.85	B	C
ATOM	2864	CG	PHE	B	133	44.883	100.013	40.520	1.00	56.97	B	C
ATOM	2865	CD1	PHE	B	133	44.244	101.132	40.014	1.00	57.99	B	C
ATOM	2866	CD2	PHE	B	133	45.699	100.158	41.626	1.00	59.08	B	C
ATOM	2867	CE1	PHE	B	133	44.416	102.367	40.603	1.00	59.29	B	C
ATOM	2868	CE2	PHE	B	133	45.875	101.389	42.217	1.00	59.51	B	C
ATOM	2869	CZ	PHE	B	133	45.236	102.492	41.709	1.00	60.13	B	C
ATOM	2870	C	PHE	B	133	46.935	99.061	38.807	1.00	41.38	B	C
ATOM	2871	O	PHE	B	133	47.511	98.860	39.859	1.00	42.52	B	O
ATOM	2872	N	TYR	B	134	47.479	99.777	37.831	1.00	31.69	B	N
ATOM	2873	CA	TYR	B	134	48.801	100.355	38.015	1.00	32.40	B	C
ATOM	2874	CB	TYR	B	134	49.362	100.939	36.724	1.00	55.82	B	C
ATOM	2875	CG	TYR	B	134	49.384	99.981	35.570	1.00	56.72	B	C

ATOM	2876	CD1	TYR	B	134	48.416	100.052	34.572	1.00	56.71	B	C
ATOM	2877	CE1	TYR	B	134	48.416	99.176	33.511	1.00	55.78	B	C
ATOM	2878	CD2	TYR	B	134	50.359	98.999	35.475	1.00	56.90	B	C
ATOM	2879	CE2	TYR	B	134	50.369	98.110	34.417	1.00	56.61	B	C
ATOM	2880	CZ	TYR	B	134	49.390	98.203	33.436	1.00	56.23	B	C
ATOM	2881	OH	TYR	B	134	49.358	97.303	32.390	1.00	57.35	B	O
ATOM	2882	C	TYR	B	134	48.737	101.458	39.054	1.00	33.08	B	C
ATOM	2883	O	TYR	B	134	49.550	101.490	39.975	1.00	34.33	B	O
ATOM	2884	N	GLY	B	135	47.786	102.378	38.924	1.00	40.63	B	N
ATOM	2885	CA	GLY	B	135	47.720	103.440	39.914	1.00	42.05	B	C
ATOM	2886	C	GLY	B	135	46.899	104.667	39.579	1.00	42.20	B	C
ATOM	2887	O	GLY	B	135	46.535	104.902	38.420	1.00	41.42	B	O
ATOM	2888	N	ALA	B	136	46.624	105.446	40.627	1.00	65.81	B	N
ATOM	2889	CA	ALA	B	136	45.835	106.677	40.548	1.00	67.71	B	C
ATOM	2890	CB	ALA	B	136	44.483	106.485	41.243	1.00	19.66	B	C
ATOM	2891	C	ALA	B	136	46.594	107.815	41.211	1.00	67.49	B	C
ATOM	2892	O	ALA	B	136	47.515	107.581	41.989	1.00	68.30	B	O
ATOM	2893	N	PHE	B	137	46.194	109.046	40.915	1.00	74.77	B	N
ATOM	2894	CA	PHE	B	137	46.872	110.204	41.475	1.00	76.02	B	C
ATOM	2895	CB	PHE	B	137	48.246	110.353	40.834	1.00	53.43	B	C
ATOM	2896	CG	PHE	B	137	48.229	110.274	39.331	1.00	51.94	B	C
ATOM	2897	CD1	PHE	B	137	48.111	109.051	38.685	1.00	50.57	B	C
ATOM	2898	CD2	PHE	B	137	48.374	111.412	38.564	1.00	51.37	B	C
ATOM	2899	CE1	PHE	B	137	48.148	108.967	37.306	1.00	51.53	B	C
ATOM	2900	CE2	PHE	B	137	48.410	111.329	37.183	1.00	51.44	B	C
ATOM	2901	CZ	PHE	B	137	48.298	110.106	36.558	1.00	50.94	B	C
ATOM	2902	C	PHE	B	137	46.112	111.503	41.282	1.00	78.88	B	C
ATOM	2903	O	PHE	B	137	45.292	111.614	40.379	1.00	78.79	B	O
ATOM	2904	N	TYR	B	138	46.411	112.488	42.128	1.00	86.27	B	N
ATOM	2905	CA	TYR	B	138	45.773	113.803	42.061	1.00	89.13	B	C
ATOM	2906	CB	TYR	B	138	46.358	114.773	43.096	1.00	203.67	B	C
ATOM	2907	CG	TYR	B	138	46.589	114.245	44.495	1.00	203.67	B	C
ATOM	2908	CD1	TYR	B	138	47.369	113.117	44.721	1.00	203.67	B	C
ATOM	2909	CE1	TYR	B	138	47.656	112.691	46.006	1.00	203.67	B	C
ATOM	2910	CD2	TYR	B	138	46.097	114.930	45.599	1.00	203.67	B	C
ATOM	2911	CE2	TYR	B	138	46.379	114.513	46.886	1.00	203.67	B	C
ATOM	2912	CZ	TYR	B	138	47.161	113.394	47.084	1.00	203.67	B	C
ATOM	2913	OH	TYR	B	138	47.461	112.986	48.364	1.00	203.67	B	O
ATOM	2914	C	TYR	B	138	46.065	114.406	40.693	1.00	91.58	B	C
ATOM	2915	O	TYR	B	138	46.619	113.749	39.816	1.00	91.33	B	O
ATOM	2916	N	SER	B	139	45.708	115.677	40.548	1.00	107.14	B	N
ATOM	2917	CA	SER	B	139	45.941	116.441	39.329	1.00	109.34	B	C
ATOM	2918	CB	SER	B	139	45.903	115.550	38.085	1.00	85.34	B	C

ATOM	2919	OG	SER	B	139	46.204	116.303	36.920	1.00 85.66	B	O
ATOM	2920	C	SER	B	139	44.911	117.544	39.178	1.00109.63	B	C
ATOM	2921	O	SER	B	139	43.874	117.547	39.846	1.00109.62	B	O
ATOM	2922	N	ASP	B	140	45.211	118.490	38.297	1.00174.14	B	N
ATOM	2923	CA	ASP	B	140	44.307	119.594	38.042	1.00174.94	B	C
ATOM	2924	CB	ASP	B	140	45.090	120.829	37.590	1.00164.55	B	C
ATOM	2925	CG	ASP	B	140	46.124	121.272	38.614	1.00166.51	B	C
ATOM	2926	OD1	ASP	B	140	45.776	121.384	39.810	1.00166.92	B	O
ATOM	2927	OD2	ASP	B	140	47.284	121.518	38.222	1.00168.12	B	O
ATOM	2928	C	ASP	B	140	43.347	119.146	36.950	1.00174.01	B	C
ATOM	2929	O	ASP	B	140	42.131	119.136	37.141	1.00174.03	B	O
ATOM	2930	N	GLY	B	141	43.903	118.759	35.808	1.00141.71	B	N
ATOM	2931	CA	GLY	B	141	43.072	118.305	34.713	1.00139.69	B	C
ATOM	2932	C	GLY	B	141	42.349	117.007	35.035	1.00137.49	B	C
ATOM	2933	O	GLY	B	141	41.353	116.679	34.390	1.00138.57	B	O
ATOM	2934	N	GLU	B	142	42.838	116.270	36.033	1.00 99.50	B	N
ATOM	2935	CA	GLU	B	142	42.221	115.000	36.408	1.00 95.65	B	C
ATOM	2936	CB	GLU	B	142	42.538	113.938	35.356	1.00152.49	B	C
ATOM	2937	CG	GLU	B	142	44.022	113.625	35.196	1.00153.65	B	C
ATOM	2938	CD	GLU	B	142	44.755	114.625	34.319	1.00154.02	B	C
ATOM	2939	OE1	GLU	B	142	44.996	115.765	34.766	1.00154.25	B	O
ATOM	2940	OE2	GLU	B	142	45.088	114.265	33.170	1.00153.93	B	O
ATOM	2941	C	GLU	B	142	42.624	114.458	37.782	1.00 92.51	B	C
ATOM	2942	O	GLU	B	142	43.233	115.157	38.589	1.00 92.39	B	O
ATOM	2943	N	ILE	B	143	42.261	113.199	38.027	1.00162.15	B	N
ATOM	2944	CA	ILE	B	143	42.560	112.500	39.279	1.00157.81	B	C
ATOM	2945	CB	ILE	B	143	41.300	112.291	40.125	1.00 51.10	B	C
ATOM	2946	CG2	ILE	B	143	40.472	111.158	39.525	1.00 49.14	B	C
ATOM	2947	CG1	ILE	B	143	41.684	111.959	41.572	1.00 52.62	B	C
ATOM	2948	CD1	ILE	B	143	40.493	111.647	42.475	1.00 55.89	B	C
ATOM	2949	C	ILE	B	143	43.092	111.124	38.900	1.00155.71	B	C
ATOM	2950	O	ILE	B	143	43.481	110.329	39.752	1.00153.48	B	O
ATOM	2951	N	SER	B	144	43.064	110.862	37.600	1.00100.59	B	N
ATOM	2952	CA	SER	B	144	43.542	109.627	36.989	1.00100.16	B	C
ATOM	2953	CB	SER	B	144	44.937	109.854	36.406	1.00 46.31	B	C
ATOM	2954	OG	SER	B	144	44.906	110.792	35.355	1.00 47.80	B	O
ATOM	2955	C	SER	B	144	43.585	108.324	37.774	1.00 98.20	B	C
ATOM	2956	O	SER	B	144	43.967	108.279	38.942	1.00 97.56	B	O
ATOM	2957	N	ILE	B	145	43.196	107.261	37.080	1.00 77.44	B	N
ATOM	2958	CA	ILE	B	145	43.224	105.899	37.593	1.00 76.45	B	C
ATOM	2959	CB	ILE	B	145	41.855	105.408	38.137	1.00 40.95	B	C
ATOM	2960	CG2	ILE	B	145	41.898	103.899	38.329	1.00 41.49	B	C
ATOM	2961	CG1	ILE	B	145	41.534	106.093	39.476	1.00 40.40	B	C

ATOM	2962	CD1	ILE	B	145	40.240	105.605	40.159	1.00	39.60	B C
ATOM	2963	C	ILE	B	145	43.626	105.043	36.392	1.00	75.85	B C
ATOM	2964	O	ILE	B	145	42.790	104.618	35.594	1.00	74.45	B O
ATOM	2965	N	CYS	B	146	44.930	104.836	36.256	1.00	49.38	B N
ATOM	2966	CA	CYS	B	146	45.481	104.043	35.176	1.00	53.10	B C
ATOM	2967	CB	CYS	B	146	46.918	104.484	34.916	1.00	77.23	B C
ATOM	2968	SG	CYS	B	146	47.188	106.229	35.296	1.00	80.97	B S
ATOM	2969	C	CYS	B	146	45.442	102.588	35.637	1.00	53.38	B C
ATOM	2970	O	CYS	B	146	45.830	102.281	36.763	1.00	54.24	B O
ATOM	2971	N	MET	B	147	44.972	101.707	34.760	1.00	44.34	B N
ATOM	2972	CA	MET	B	147	44.843	100.289	35.065	1.00	44.63	B C
ATOM	2973	CB	MET	B	147	43.408	99.995	35.500	1.00	102.48	B C
ATOM	2974	CG	MET	B	147	42.366	100.537	34.532	1.00	105.34	B C
ATOM	2975	SD	MET	B	147	40.668	100.258	35.060	1.00	109.77	B S
ATOM	2976	CE	MET	B	147	40.000	99.420	33.647	1.00	108.61	B C
ATOM	2977	C	MET	B	147	45.190	99.417	33.866	1.00	43.00	B C
ATOM	2978	O	MET	B	147	45.591	99.916	32.821	1.00	42.91	B O
ATOM	2979	N	GLU	B	148	45.008	98.111	34.008	1.00	45.57	B N
ATOM	2980	CA	GLU	B	148	45.329	97.194	32.924	1.00	43.97	B C
ATOM	2981	CB	GLU	B	148	45.185	95.739	33.384	1.00	51.13	B C
ATOM	2982	CG	GLU	B	148	44.739	94.790	32.265	1.00	51.97	B C
ATOM	2983	CD	GLU	B	148	44.794	93.328	32.658	1.00	52.62	B C
ATOM	2984	OE1	GLU	B	148	44.425	92.994	33.803	1.00	49.12	B O
ATOM	2985	OE2	GLU	B	148	45.195	92.507	31.812	1.00	53.73	B O
ATOM	2986	C	GLU	B	148	44.522	97.381	31.647	1.00	42.76	B C
ATOM	2987	O	GLU	B	148	43.294	97.394	31.664	1.00	43.96	B O
ATOM	2988	N	HIS	B	149	45.234	97.498	30.532	1.00	42.26	B N
ATOM	2989	CA	HIS	B	149	44.605	97.655	29.229	1.00	41.36	B C
ATOM	2990	CB	HIS	B	149	45.645	98.120	28.211	1.00	73.73	B C
ATOM	2991	CG	HIS	B	149	45.070	98.467	26.875	1.00	70.58	B C
ATOM	2992	CD2	HIS	B	149	45.323	99.499	26.039	1.00	67.79	B C
ATOM	2993	ND1	HIS	B	149	44.129	97.685	26.243	1.00	68.83	B N
ATOM	2994	CE1	HIS	B	149	43.824	98.221	25.077	1.00	66.70	B C
ATOM	2995	NE2	HIS	B	149	44.536	99.322	24.928	1.00	64.57	B N
ATOM	2996	C	HIS	B	149	44.003	96.322	28.773	1.00	42.73	B C
ATOM	2997	O	HIS	B	149	44.587	95.267	28.997	1.00	45.05	B O
ATOM	2998	N	MET	B	150	42.835	96.380	28.134	1.00	30.49	B N
ATOM	2999	CA	MET	B	150	42.150	95.187	27.632	1.00	31.31	B C
ATOM	3000	CB	MET	B	150	40.810	95.011	28.353	1.00	68.97	B C
ATOM	3001	CG	MET	B	150	40.898	95.034	29.886	1.00	70.32	B C
ATOM	3002	SD	MET	B	150	41.909	93.727	30.667	1.00	72.78	B S
ATOM	3003	CE	MET	B	150	40.852	92.291	30.449	1.00	69.92	B C
ATOM	3004	C	MET	B	150	41.919	95.277	26.119	1.00	30.64	B C

ATOM	3005	O	MET	B	150	41.400	96.277	25.629	1.00	29.96	B	O
ATOM	3006	N	ASP	B	151	42.321	94.232	25.395	1.00	47.67	B	N
ATOM	3007	CA	ASP	B	151	42.166	94.171	23.943	1.00	48.65	B	C
ATOM	3008	CB	ASP	B	151	42.665	92.844	23.386	1.00	87.39	B	C
ATOM	3009	CG	ASP	B	151	44.090	92.575	23.740	1.00	89.35	B	C
ATOM	3010	OD1	ASP	B	151	44.331	92.083	24.856	1.00	88.68	B	O
ATOM	3011	OD2	ASP	B	151	44.973	92.864	22.908	1.00	91.39	B	O
ATOM	3012	C	ASP	B	151	40.710	94.318	23.575	1.00	50.50	B	C
ATOM	3013	O	ASP	B	151	40.367	94.988	22.601	1.00	50.60	B	O
ATOM	3014	N	GLY	B	152	39.854	93.647	24.331	1.00	71.87	B	N
ATOM	3015	CA	GLY	B	152	38.439	93.773	24.078	1.00	72.90	B	C
ATOM	3016	C	GLY	B	152	38.044	95.047	24.797	1.00	74.77	B	C
ATOM	3017	O	GLY	B	152	38.898	95.788	25.290	1.00	76.05	B	O
ATOM	3018	N	GLY	B	153	36.755	95.322	24.866	1.00	72.72	B	N
ATOM	3019	CA	GLY	B	153	36.334	96.517	25.559	1.00	71.80	B	C
ATOM	3020	C	GLY	B	153	35.144	96.134	26.395	1.00	72.30	B	C
ATOM	3021	O	GLY	B	153	34.891	94.945	26.578	1.00	74.05	B	O
ATOM	3022	N	SER	B	154	34.419	97.122	26.906	1.00	38.65	B	N
ATOM	3023	CA	SER	B	154	33.246	96.832	27.697	1.00	38.40	B	C
ATOM	3024	CB	SER	B	154	32.416	98.096	27.893	1.00	96.55	B	C
ATOM	3025	OG	SER	B	154	33.002	98.938	28.866	1.00	99.49	B	O
ATOM	3026	C	SER	B	154	32.464	95.784	26.922	1.00	36.64	B	C
ATOM	3027	O	SER	B	154	32.230	95.943	25.733	1.00	35.70	B	O
ATOM	3028	N	LEU	B	155	32.089	94.701	27.592	1.00	42.20	B	N
ATOM	3029	CA	LEU	B	155	31.355	93.642	26.937	1.00	43.59	B	C
ATOM	3030	CB	LEU	B	155	30.749	92.714	27.986	1.00	18.62	B	C
ATOM	3031	CG	LEU	B	155	31.346	91.305	28.187	1.00	20.07	B	C
ATOM	3032	CD1	LEU	B	155	30.274	90.433	28.857	1.00	19.52	B	C
ATOM	3033	CD2	LEU	B	155	31.777	90.663	26.864	1.00	20.46	B	C
ATOM	3034	C	LEU	B	155	30.274	94.156	25.966	1.00	44.72	B	C
ATOM	3035	O	LEU	B	155	30.046	93.562	24.911	1.00	45.91	B	O
ATOM	3036	N	ASP	B	156	29.603	95.253	26.290	1.00	60.92	B	N
ATOM	3037	CA	ASP	B	156	28.604	95.742	25.348	1.00	58.41	B	C
ATOM	3038	CB	ASP	B	156	27.879	96.976	25.874	1.00	36.48	B	C
ATOM	3039	CG	ASP	B	156	28.813	98.094	26.179	1.00	37.73	B	C
ATOM	3040	OD1	ASP	B	156	28.353	99.253	26.170	1.00	38.92	B	O
ATOM	3041	OD2	ASP	B	156	29.997	97.803	26.434	1.00	38.19	B	O
ATOM	3042	C	ASP	B	156	29.326	96.089	24.054	1.00	56.32	B	C
ATOM	3043	O	ASP	B	156	28.786	95.898	22.974	1.00	57.39	B	O
ATOM	3044	N	GLN	B	157	30.542	96.612	24.163	1.00	51.52	B	N
ATOM	3045	CA	GLN	B	157	31.317	96.927	22.971	1.00	52.75	B	C
ATOM	3046	CB	GLN	B	157	32.761	97.260	23.315	1.00	53.06	B	C
ATOM	3047	CG	GLN	B	157	32.999	98.609	23.916	1.00	55.48	B	C

ATOM	3048	CD	GLN	B	157	34.454	98.993	23.796	1.00	57.68	B	C
ATOM	3049	OE1	GLN	B	157	35.050	98.831	22.736	1.00	59.57	B	O
ATOM	3050	NE2	GLN	B	157	35.036	99.503	24.869	1.00	59.20	B	N
ATOM	3051	C	GLN	B	157	31.329	95.682	22.101	1.00	51.27	B	C
ATOM	3052	O	GLN	B	157	30.806	95.674	20.989	1.00	49.84	B	O
ATOM	3053	N	VAL	B	158	31.941	94.623	22.615	1.00	65.04	B	N
ATOM	3054	CA	VAL	B	158	32.013	93.380	21.874	1.00	65.28	B	C
ATOM	3055	CB	VAL	B	158	32.582	92.250	22.740	1.00	73.04	B	C
ATOM	3056	CG1	VAL	B	158	33.649	92.808	23.661	1.00	73.22	B	C
ATOM	3057	CG2	VAL	B	158	31.478	91.579	23.522	1.00	72.22	B	C
ATOM	3058	C	VAL	B	158	30.601	93.036	21.441	1.00	64.25	B	C
ATOM	3059	O	VAL	B	158	30.391	92.484	20.369	1.00	63.28	B	O
ATOM	3060	N	LEU	B	159	29.626	93.382	22.272	1.00	61.25	B	N
ATOM	3061	CA	LEU	B	159	28.243	93.106	21.924	1.00	61.69	B	C
ATOM	3062	CB	LEU	B	159	27.305	93.466	23.082	1.00	32.63	B	C
ATOM	3063	CG	LEU	B	159	25.823	93.279	22.747	1.00	30.78	B	C
ATOM	3064	CD1	LEU	B	159	25.665	92.117	21.807	1.00	29.74	B	C
ATOM	3065	CD2	LEU	B	159	25.016	93.051	24.010	1.00	31.26	B	C
ATOM	3066	C	LEU	B	159	27.903	93.937	20.702	1.00	61.14	B	C
ATOM	3067	O	LEU	B	159	27.395	93.422	19.704	1.00	61.72	B	O
ATOM	3068	N	LYS	B	160	28.197	95.229	20.796	1.00	86.49	B	N
ATOM	3069	CA	LYS	B	160	27.941	96.167	19.717	1.00	88.86	B	C
ATOM	3070	CB	LYS	B	160	28.729	97.460	19.940	1.00	120.57	B	C
ATOM	3071	CG	LYS	B	160	28.830	98.360	18.716	1.00	122.54	B	C
ATOM	3072	CD	LYS	B	160	27.469	98.875	18.265	1.00	124.52	B	C
ATOM	3073	CE	LYS	B	160	27.589	99.769	17.030	1.00	124.74	B	C
ATOM	3074	NZ	LYS	B	160	26.274	100.326	16.594	1.00	126.98	B	N
ATOM	3075	C	LYS	B	160	28.332	95.553	18.391	1.00	90.76	B	C
ATOM	3076	O	LYS	B	160	27.583	95.634	17.424	1.00	90.20	B	O
ATOM	3077	N	GLU	B	161	29.497	94.916	18.351	1.00	89.91	B	N
ATOM	3078	CA	GLU	B	161	29.965	94.310	17.114	1.00	89.42	B	C
ATOM	3079	CB	GLU	B	161	31.429	94.696	16.875	1.00	77.68	B	C
ATOM	3080	CG	GLU	B	161	31.586	96.108	16.339	1.00	82.77	B	C
ATOM	3081	CD	GLU	B	161	33.017	96.460	15.989	1.00	86.00	B	C
ATOM	3082	OE1	GLU	B	161	33.816	96.695	16.917	1.00	87.41	B	O
ATOM	3083	OE2	GLU	B	161	33.347	96.500	14.785	1.00	87.10	B	O
ATOM	3084	C	GLU	B	161	29.798	92.796	16.984	1.00	88.06	B	C
ATOM	3085	O	GLU	B	161	30.507	92.165	16.198	1.00	87.89	B	O
ATOM	3086	N	ALA	B	162	28.853	92.216	17.723	1.00	29.74	B	N
ATOM	3087	CA	ALA	B	162	28.628	90.774	17.668	1.00	29.74	B	C
ATOM	3088	CB	ALA	B	162	29.389	90.086	18.764	1.00	37.59	B	C
ATOM	3089	C	ALA	B	162	27.166	90.436	17.785	1.00	28.28	B	C
ATOM	3090	O	ALA	B	162	26.793	89.278	17.684	1.00	26.85	B	O

ATOM	3091	N	LYS	B	163	26.352	91.460	18.017	1.00	69.62	B	N
ATOM	3092	CA	LYS	B	163	24.903	91.326	18.132	1.00	68.97	B	C
ATOM	3093	CB	LYS	B	163	24.285	91.225	16.733	1.00	77.40	B	C
ATOM	3094	CG	LYS	B	163	24.857	92.217	15.726	1.00	79.20	B	C
ATOM	3095	CD	LYS	B	163	24.846	93.670	16.234	1.00	81.84	B	C
ATOM	3096	CE	LYS	B	163	23.450	94.303	16.213	1.00	80.60	B	C
ATOM	3097	NZ	LYS	B	163	23.466	95.750	16.598	1.00	80.38	B	N
ATOM	3098	C	LYS	B	163	24.420	90.151	18.981	1.00	67.93	B	C
ATOM	3099	O	LYS	B	163	23.584	89.369	18.535	1.00	68.03	B	O
ATOM	3100	N	ARG	B	164	24.960	90.062	20.195	1.00	53.65	B	N
ATOM	3101	CA	ARG	B	164	24.679	89.055	21.231	1.00	50.96	B	C
ATOM	3102	CB	ARG	B	164	23.218	88.542	21.208	1.00	59.67	B	C
ATOM	3103	CG	ARG	B	164	22.765	87.620	20.078	1.00	64.06	B	C
ATOM	3104	CD	ARG	B	164	23.423	86.253	20.044	1.00	64.90	B	C
ATOM	3105	NE	ARG	B	164	24.745	86.300	19.429	1.00	66.30	B	N
ATOM	3106	CZ	ARG	B	164	25.330	85.273	18.819	1.00	66.14	B	C
ATOM	3107	NH1	ARG	B	164	24.705	84.104	18.732	1.00	65.75	B	N
ATOM	3108	NH2	ARG	B	164	26.548	85.408	18.306	1.00	65.50	B	N
ATOM	3109	C	ARG	B	164	25.613	87.876	21.297	1.00	46.93	B	C
ATOM	3110	O	ARG	B	164	26.409	87.629	20.399	1.00	48.89	B	O
ATOM	3111	N	ILE	B	165	25.512	87.165	22.407	1.00	54.63	B	N
ATOM	3112	CA	ILE	B	165	26.322	85.997	22.653	1.00	49.92	B	C
ATOM	3113	CB	ILE	B	165	27.155	86.151	23.898	1.00	21.60	B	C
ATOM	3114	CG2	ILE	B	165	28.576	85.870	23.541	1.00	21.19	B	C
ATOM	3115	CG1	ILE	B	165	27.113	87.588	24.413	1.00	21.19	B	C
ATOM	3116	CD1	ILE	B	165	27.922	88.564	23.579	1.00	21.19	B	C
ATOM	3117	C	ILE	B	165	25.368	84.817	22.804	1.00	48.92	B	C
ATOM	3118	O	ILE	B	165	24.152	84.996	22.896	1.00	48.92	B	O
ATOM	3119	N	PRO	B	166	25.885	83.583	22.856	1.00	48.95	B	N
ATOM	3120	CD	PRO	B	166	25.991	84.006	21.448	1.00	63.42	B	C
ATOM	3121	CA	PRO	B	166	26.706	82.389	22.884	1.00	50.27	B	C
ATOM	3122	CB	PRO	B	166	28.002	82.872	22.285	1.00	63.13	B	C
ATOM	3123	CG	PRO	B	166	27.453	83.608	21.061	1.00	63.41	B	C
ATOM	3124	C	PRO	B	166	26.796	81.825	24.277	1.00	51.66	B	C
ATOM	3125	O	PRO	B	166	27.780	81.999	24.987	1.00	54.37	B	O
ATOM	3126	N	GLU	B	167	25.712	81.130	24.644	1.00	37.46	B	N
ATOM	3127	CA	GLU	B	167	25.578	80.534	25.941	1.00	37.09	B	C
ATOM	3128	CB	GLU	B	167	24.633	79.349	25.886	1.00	26.69	B	C
ATOM	3129	CG	GLU	B	167	24.306	78.813	27.244	1.00	26.86	B	C
ATOM	3130	CD	GLU	B	167	23.120	77.884	27.228	1.00	27.04	B	C
ATOM	3131	OE1	GLU	B	167	22.067	78.294	26.698	1.00	29.79	B	O
ATOM	3132	OE2	GLU	B	167	23.232	76.752	27.749	1.00	27.90	B	O
ATOM	3133	C	GLU	B	167	26.911	80.120	26.515	1.00	37.71	B	C

ATOM	3134	O	GLU	B	167	27.390	80.761	27.450	1.00	37.10	B	O
ATOM	3135	N	GLU	B	168	27.541	79.092	25.949	1.00	50.86	B	N
ATOM	3136	CA	GLU	B	168	28.814	78.637	26.504	1.00	53.83	B	C
ATOM	3137	CB	GLU	B	168	29.458	77.556	25.632	1.00	71.15	B	C
ATOM	3138	CG	GLU	B	168	30.122	76.400	26.447	1.00	79.44	B	C
ATOM	3139	CD	GLU	B	168	29.149	75.618	27.354	1.00	85.30	B	C
ATOM	3140	OE1	GLU	B	168	29.440	74.443	27.681	1.00	89.07	B	O
ATOM	3141	OE2	GLU	B	168	28.103	76.172	27.753	1.00	89.39	B	O
ATOM	3142	C	GLU	B	168	29.756	79.808	26.721	1.00	52.22	B	C
ATOM	3143	O	GLU	B	168	30.525	79.814	27.686	1.00	53.53	B	O
ATOM	3144	N	ILE	B	169	29.686	80.806	25.844	1.00	47.66	B	N
ATOM	3145	CA	ILE	B	169	30.510	81.993	26.021	1.00	45.85	B	C
ATOM	3146	CB	ILE	B	169	30.385	82.997	24.862	1.00	43.49	B	C
ATOM	3147	CG2	ILE	B	169	30.865	84.370	25.320	1.00	42.91	B	C
ATOM	3148	CG1	ILE	B	169	31.273	82.570	23.706	1.00	42.69	B	C
ATOM	3149	CD1	ILE	B	169	32.752	82.590	24.076	1.00	41.26	B	C
ATOM	3150	C	ILE	B	169	30.027	82.700	27.278	1.00	45.37	B	C
ATOM	3151	O	ILE	B	169	30.780	82.861	28.241	1.00	43.85	B	O
ATOM	3152	N	LEU	B	170	28.765	83.126	27.266	1.00	32.65	B	N
ATOM	3153	CA	LEU	B	170	28.200	83.808	28.417	1.00	33.66	B	C
ATOM	3154	CB	LEU	B	170	26.741	84.141	28.158	1.00	35.12	B	C
ATOM	3155	CG	LEU	B	170	26.653	85.313	27.184	1.00	35.73	B	C
ATOM	3156	CD1	LEU	B	170	25.257	85.910	27.245	1.00	35.45	B	C
ATOM	3157	CD2	LEU	B	170	27.708	86.362	27.543	1.00	33.98	B	C
ATOM	3158	C	LEU	B	170	28.351	82.961	29.674	1.00	34.02	B	C
ATOM	3159	O	LEU	B	170	28.339	83.473	30.799	1.00	36.20	B	O
ATOM	3160	N	GLY	B	171	28.487	81.656	29.473	1.00	25.65	B	N
ATOM	3161	CA	GLY	B	171	28.701	80.757	30.586	1.00	24.82	B	C
ATOM	3162	C	GLY	B	171	30.146	80.969	30.998	1.00	24.45	B	C
ATOM	3163	O	GLY	B	171	30.490	80.915	32.164	1.00	23.46	B	O
ATOM	3164	N	LYS	B	172	31.013	81.215	30.033	1.00	39.28	B	N
ATOM	3165	CA	LYS	B	172	32.393	81.454	30.387	1.00	39.59	B	C
ATOM	3166	CB	LYS	B	172	33.284	81.509	29.145	1.00	35.96	B	C
ATOM	3167	CG	LYS	B	172	34.203	80.318	28.982	1.00	38.30	B	C
ATOM	3168	CD	LYS	B	172	35.553	80.752	28.435	1.00	40.67	B	C
ATOM	3169	CE	LYS	B	172	36.263	81.735	29.378	1.00	40.42	B	C
ATOM	3170	NZ	LYS	B	172	37.752	81.840	29.156	1.00	41.32	B	N
ATOM	3171	C	LYS	B	172	32.460	82.788	31.108	1.00	39.00	B	C
ATOM	3172	O	LYS	B	172	33.416	83.055	31.835	1.00	40.85	B	O
ATOM	3173	N	VAL	B	173	31.439	83.619	30.904	1.00	36.11	B	N
ATOM	3174	CA	VAL	B	173	31.380	84.945	31.519	1.00	35.66	B	C
ATOM	3175	CB	VAL	B	173	30.524	85.904	30.691	1.00	43.16	B	C
ATOM	3176	CG1	VAL	B	173	30.421	87.240	31.396	1.00	44.30	B	C

ATOM	3177	CG2	VAL	B	173	31.124	86.072	29.322	1.00	44.06	B	C
ATOM	3178	C	VAL	B	173	30.820	84.949	32.931	1.00	35.45	B	C
ATOM	3179	O	VAL	B	173	31.236	85.741	33.771	1.00	35.15	B	O
ATOM	3180	N	SER	B	174	29.858	84.081	33.193	1.00	38.94	B	N
ATOM	3181	CA	SER	B	174	29.281	84.021	34.518	1.00	39.23	B	C
ATOM	3182	CB	SER	B	174	28.153	82.991	34.530	1.00	36.15	B	C
ATOM	3183	OG	SER	B	174	27.279	83.203	33.429	1.00	36.15	B	O
ATOM	3184	C	SER	B	174	30.407	83.643	35.480	1.00	38.67	B	C
ATOM	3185	O	SER	B	174	30.639	84.313	36.487	1.00	38.67	B	O
ATOM	3186	N	ILE	B	175	31.114	82.571	35.152	1.00	37.40	B	N
ATOM	3187	CA	ILE	B	175	32.242	82.117	35.953	1.00	37.40	B	C
ATOM	3188	CB	ILE	B	175	33.092	81.099	35.174	1.00	17.11	B	C
ATOM	3189	CG2	ILE	B	175	34.416	80.885	35.873	1.00	16.61	B	C
ATOM	3190	CG1	ILE	B	175	32.305	79.804	34.974	1.00	19.44	B	C
ATOM	3191	CD1	ILE	B	175	32.864	78.930	33.862	1.00	21.42	B	C
ATOM	3192	C	ILE	B	175	33.143	83.300	36.302	1.00	37.50	B	C
ATOM	3193	O	ILE	B	175	33.641	83.403	37.410	1.00	37.40	B	O
ATOM	3194	N	ALA	B	176	33.361	84.193	35.348	1.00	23.37	B	N
ATOM	3195	CA	ALA	B	176	34.215	85.355	35.578	1.00	23.26	B	C
ATOM	3196	CB	ALA	B	176	34.423	86.103	34.270	1.00	78.62	B	C
ATOM	3197	C	ALA	B	176	33.643	86.301	36.638	1.00	23.26	B	C
ATOM	3198	O	ALA	B	176	34.154	86.392	37.753	1.00	23.26	B	O
ATOM	3199	N	VAL	B	177	32.588	87.017	36.269	1.00	37.32	B	N
ATOM	3200	CA	VAL	B	177	31.932	87.949	37.175	1.00	37.32	B	C
ATOM	3201	CB	VAL	B	177	30.584	88.409	36.593	1.00	20.71	B	C
ATOM	3202	CG1	VAL	B	177	29.766	89.107	37.659	1.00	20.71	B	C
ATOM	3203	CG2	VAL	B	177	30.826	89.329	35.428	1.00	20.71	B	C
ATOM	3204	C	VAL	B	177	31.675	87.285	38.521	1.00	37.32	B	C
ATOM	3205	O	VAL	B	177	32.091	87.777	39.568	1.00	37.32	B	O
ATOM	3206	N	LEU	B	178	30.987	86.152	38.463	1.00	33.82	B	N
ATOM	3207	CA	LEU	B	178	30.630	85.388	39.637	1.00	35.18	B	C
ATOM	3208	CB	LEU	B	178	29.992	84.076	39.183	1.00	8.43	B	C
ATOM	3209	CG	LEU	B	178	28.876	83.458	40.027	1.00	9.35	B	C
ATOM	3210	CD1	LEU	B	178	27.983	84.515	40.640	1.00	7.90	B	C
ATOM	3211	CD2	LEU	B	178	28.073	82.547	39.144	1.00	9.69	B	C
ATOM	3212	C	LEU	B	178	31.863	85.140	40.507	1.00	35.27	B	C
ATOM	3213	O	LEU	B	178	31.788	85.115	41.736	1.00	36.09	B	O
ATOM	3214	N	ARG	B	179	33.012	84.969	39.871	1.00	21.12	B	N
ATOM	3215	CA	ARG	B	179	34.224	84.723	40.625	1.00	22.82	B	C
ATOM	3216	CB	ARG	B	179	35.247	84.007	39.749	1.00	55.33	B	C
ATOM	3217	CG	ARG	B	179	36.089	83.016	40.509	1.00	58.46	B	C
ATOM	3218	CD	ARG	B	179	36.779	82.000	39.590	1.00	62.14	B	C
ATOM	3219	NE	ARG	B	179	35.878	81.022	38.978	1.00	66.30	B	N

ATOM	3220	CZ	ARG	B	179	36.280	79.838	38.522	1.00	68.61	B	C
ATOM	3221	NH1	ARG	B	179	35.413	78.995	37.978	1.00	71.14	B	N
ATOM	3222	NH2	ARG	B	179	37.557	79.495	38.622	1.00	68.43	B	N
ATOM	3223	C	ARG	B	179	34.737	86.071	41.081	1.00	21.93	B	C
ATOM	3224	O	ARG	B	179	34.951	86.294	42.263	1.00	23.16	B	O
ATOM	3225	N	GLY	B	180	34.910	86.982	40.136	1.00	24.73	B	N
ATOM	3226	CA	GLY	B	180	35.375	88.303	40.494	1.00	24.31	B	C
ATOM	3227	C	GLY	B	180	34.492	88.862	41.588	1.00	22.88	B	C
ATOM	3228	O	GLY	B	180	34.972	89.536	42.491	1.00	22.60	B	O
ATOM	3229	N	LEU	B	181	33.200	88.563	41.513	1.00	23.51	B	N
ATOM	3230	CA	LEU	B	181	32.229	89.042	42.494	1.00	23.91	B	C
ATOM	3231	CB	LEU	B	181	30.835	88.515	42.152	1.00	21.40	B	C
ATOM	3232	CG	LEU	B	181	29.711	89.554	42.064	1.00	22.49	B	C
ATOM	3233	CD1	LEU	B	181	30.292	90.951	41.952	1.00	23.38	B	C
ATOM	3234	CD2	LEU	B	181	28.824	89.247	40.866	1.00	21.40	B	C
ATOM	3235	C	LEU	B	181	32.609	88.616	43.902	1.00	23.76	B	C
ATOM	3236	O	LEU	B	181	32.642	89.436	44.822	1.00	24.06	B	O
ATOM	3237	N	ALA	B	182	32.907	87.329	44.060	1.00	22.74	B	N
ATOM	3238	CA	ALA	B	182	33.295	86.777	45.353	1.00	23.33	B	C
ATOM	3239	CB	ALA	B	182	33.144	85.284	45.340	1.00	7.18	B	C
ATOM	3240	C	ALA	B	182	34.722	87.148	45.738	1.00	22.73	B	C
ATOM	3241	O	ALA	B	182	35.062	87.172	46.908	1.00	23.40	B	O
ATOM	3242	N	TYR	B	183	35.572	87.424	44.766	1.00	18.05	B	N
ATOM	3243	CA	TYR	B	183	36.920	87.806	45.123	1.00	19.57	B	C
ATOM	3244	CB	TYR	B	183	37.719	88.282	43.907	1.00	33.64	B	C
ATOM	3245	CG	TYR	B	183	39.070	88.832	44.281	1.00	33.60	B	C
ATOM	3246	CD1	TYR	B	183	40.045	88.003	44.804	1.00	33.60	B	C
ATOM	3247	CE1	TYR	B	183	41.240	88.508	45.254	1.00	33.99	B	C
ATOM	3248	CD2	TYR	B	183	39.336	90.193	44.203	1.00	33.60	B	C
ATOM	3249	CE2	TYR	B	183	40.526	90.710	44.648	1.00	34.17	B	C
ATOM	3250	CZ	TYR	B	183	41.469	89.862	45.178	1.00	34.73	B	C
ATOM	3251	OH	TYR	B	183	42.634	90.366	45.687	1.00	37.43	B	O
ATOM	3252	C	TYR	B	183	36.717	88.960	46.067	1.00	18.17	B	C
ATOM	3253	O	TYR	B	183	36.915	88.843	47.266	1.00	20.52	B	O
ATOM	3254	N	LEU	B	184	36.274	90.076	45.513	1.00	31.76	B	N
ATOM	3255	CA	LEU	B	184	36.044	91.267	46.300	1.00	32.52	B	C
ATOM	3256	CB	LEU	B	184	35.178	92.229	45.494	1.00	36.92	B	C
ATOM	3257	CG	LEU	B	184	35.749	92.565	44.108	1.00	36.47	B	C
ATOM	3258	CD1	LEU	B	184	34.749	93.408	43.353	1.00	36.21	B	C
ATOM	3259	CD2	LEU	B	184	37.068	93.300	44.221	1.00	37.30	B	C
ATOM	3260	C	LEU	B	184	35.403	90.939	47.650	1.00	35.51	B	C
ATOM	3261	O	LEU	B	184	35.908	91.342	48.699	1.00	34.69	B	O
ATOM	3262	N	ARG	B	185	34.305	90.189	47.624	1.00	23.71	B	N

ATOM	3263	CA	ARG	B	185	33.607	89.817	48.857	1.00 28.88	B	C
ATOM	3264	CB	ARG	B	185	32.505	88.796	48.594	1.00123.05	B	C
ATOM	3265	CG	ARG	B	185	31.184	89.360	48.150	1.00127.29	B	C
ATOM	3266	CD	ARG	B	185	30.076	88.522	48.761	1.00130.19	B	C
ATOM	3267	NE	ARG	B	185	29.926	88.787	50.193	1.00136.00	B	N
ATOM	3268	CZ	ARG	B	185	29.382	87.941	51.065	1.00139.17	B	C
ATOM	3269	NH1	ARG	B	185	28.940	86.758	50.658	1.00142.87	B	N
ATOM	3270	NH2	ARG	B	185	29.266	88.288	52.342	1.00140.65	B	N
ATOM	3271	C	ARG	B	185	34.541	89.221	49.878	1.00 30.63	B	C
ATOM	3272	O	ARG	B	185	34.799	89.820	50.909	1.00 31.09	B	O
ATOM	3273	N	GLU	B	186	35.035	88.024	49.584	1.00 29.62	B	N
ATOM	3274	CA	GLU	B	186	35.920	87.327	50.498	1.00 32.18	B	C
ATOM	3275	CB	GLU	B	186	36.266	85.948	49.935	1.00 79.30	B	C
ATOM	3276	CG	GLU	B	186	35.041	85.227	49.385	1.00 78.22	B	C
ATOM	3277	CD	GLU	B	186	35.325	83.810	48.923	1.00 77.04	B	C
ATOM	3278	OE1	GLU	B	186	36.449	83.551	48.446	1.00 77.28	B	O
ATOM	3279	OE2	GLU	B	186	34.414	82.959	49.018	1.00 76.49	B	O
ATOM	3280	C	GLU	B	186	37.155	88.175	50.694	1.00 33.53	B	C
ATOM	3281	O	GLU	B	186	37.642	88.790	49.748	1.00 35.44	B	O
ATOM	3282	N	LYS	B	187	37.641	88.227	51.931	1.00102.68	B	N
ATOM	3283	CA	LYS	B	187	38.824	89.014	52.275	1.00103.20	B	C
ATOM	3284	CB	LYS	B	187	40.038	88.091	52.447	1.00116.34	B	C
ATOM	3285	CG	LYS	B	187	39.930	87.156	53.665	1.00119.20	B	C
ATOM	3286	CD	LYS	B	187	39.868	87.941	54.982	1.00121.84	B	C
ATOM	3287	CE	LYS	B	187	39.499	87.059	56.182	1.00123.35	B	C
ATOM	3288	NZ	LYS	B	187	40.507	86.010	56.516	1.00126.46	B	N
ATOM	3289	C	LYS	B	187	39.104	90.113	51.245	1.00102.87	B	C
ATOM	3290	O	LYS	B	187	39.882	89.937	50.303	1.00103.52	B	O
ATOM	3291	N	HIS	B	188	38.421	91.235	51.464	1.00 53.35	B	N
ATOM	3292	CA	HIS	B	188	38.454	92.452	50.655	1.00 52.80	B	C
ATOM	3293	CB	HIS	B	188	38.660	92.153	49.173	1.00 59.25	B	C
ATOM	3294	CG	HIS	B	188	39.990	92.597	48.653	1.00 56.41	B	C
ATOM	3295	CD2	HIS	B	188	40.860	92.005	47.800	1.00 54.33	B	C
ATOM	3296	ND1	HIS	B	188	40.564	93.796	49.014	1.00 55.78	B	N
ATOM	3297	CE1	HIS	B	188	41.730	93.921	48.408	1.00 54.94	B	C
ATOM	3298	NE2	HIS	B	188	41.933	92.848	47.666	1.00 52.82	B	N
ATOM	3299	C	HIS	B	188	37.098	93.123	50.837	1.00 54.19	B	C
ATOM	3300	O	HIS	B	188	36.883	94.235	50.385	1.00 54.82	B	O
ATOM	3301	N	GLN	B	189	36.194	92.415	51.507	1.00 46.71	B	N
ATOM	3302	CA	GLN	B	189	34.837	92.865	51.799	1.00 49.28	B	C
ATOM	3303	CB	GLN	B	189	34.729	93.248	53.279	1.00114.45	B	C
ATOM	3304	CG	GLN	B	189	35.931	94.010	53.852	1.00118.63	B	C
ATOM	3305	CD	GLN	B	189	36.014	95.464	53.403	1.00122.39	B	C

ATOM	3306	OE1	GLN	B	189	36.413	95.762	52.277	1.00	123.30	B	O
ATOM	3307	NE2	GLN	B	189	35.631	96.377	54.290	1.00	123.91	B	N
ATOM	3308	C	GLN	B	189	34.301	93.996	50.950	1.00	49.43	B	C
ATOM	3309	O	GLN	B	189	33.843	94.994	51.482	1.00	49.76	B	O
ATOM	3310	N	ILE	B	190	34.329	93.855	49.634	1.00	64.77	B	N
ATOM	3311	CA	ILE	B	190	33.832	94.937	48.804	1.00	63.14	B	C
ATOM	3312	CB	ILE	B	190	34.998	95.708	48.134	1.00	72.79	B	C
ATOM	3313	CG2	ILE	B	190	35.949	94.759	47.453	1.00	74.08	B	C
ATOM	3314	CG1	ILE	B	190	34.440	96.697	47.120	1.00	74.03	B	C
ATOM	3315	CD1	ILE	B	190	33.467	97.696	47.722	1.00	75.62	B	C
ATOM	3316	C	ILE	B	190	32.814	94.539	47.745	1.00	59.91	B	C
ATOM	3317	O	ILE	B	190	33.061	93.668	46.920	1.00	58.63	B	O
ATOM	3318	N	MET	B	191	31.665	95.207	47.791	1.00	49.97	B	N
ATOM	3319	CA	MET	B	191	30.553	94.999	46.869	1.00	48.96	B	C
ATOM	3320	CB	MET	B	191	29.299	95.647	47.455	1.00	35.10	B	C
ATOM	3321	CG	MET	B	191	27.991	95.290	46.780	1.00	40.09	B	C
ATOM	3322	SD	MET	B	191	26.641	96.193	47.553	1.00	47.72	B	S
ATOM	3323	CE	MET	B	191	27.115	96.094	49.237	1.00	45.47	B	C
ATOM	3324	C	MET	B	191	30.901	95.687	45.566	1.00	46.45	B	C
ATOM	3325	O	MET	B	191	31.648	96.664	45.572	1.00	45.36	B	O
ATOM	3326	N	HIS	B	192	30.371	95.203	44.447	1.00	30.26	B	N
ATOM	3327	CA	HIS	B	192	30.670	95.858	43.177	1.00	28.88	B	C
ATOM	3328	CB	HIS	B	192	30.441	94.924	42.008	1.00	41.95	B	C
ATOM	3329	CG	HIS	B	192	31.184	95.334	40.778	1.00	38.92	B	C
ATOM	3330	CD2	HIS	B	192	31.885	94.612	39.871	1.00	39.11	B	C
ATOM	3331	ND1	HIS	B	192	31.277	96.647	40.377	1.00	37.12	B	N
ATOM	3332	CE1	HIS	B	192	32.005	96.716	39.278	1.00	37.98	B	C
ATOM	3333	NE2	HIS	B	192	32.388	95.496	38.950	1.00	38.66	B	N
ATOM	3334	C	HIS	B	192	29.805	97.102	42.994	1.00	28.27	B	C
ATOM	3335	O	HIS	B	192	30.312	98.205	42.768	1.00	29.58	B	O
ATOM	3336	N	ARG	B	193	28.492	96.908	43.090	1.00	67.52	B	N
ATOM	3337	CA	ARG	B	193	27.524	97.991	42.965	1.00	68.60	B	C
ATOM	3338	CB	ARG	B	193	27.865	99.108	43.953	1.00	79.46	B	C
ATOM	3339	CG	ARG	B	193	27.722	98.673	45.390	1.00	82.44	B	C
ATOM	3340	CD	ARG	B	193	28.344	99.643	46.374	1.00	84.93	B	C
ATOM	3341	NE	ARG	B	193	28.595	98.959	47.642	1.00	89.03	B	N
ATOM	3342	CZ	ARG	B	193	29.215	99.493	48.690	1.00	89.92	B	C
ATOM	3343	NH1	ARG	B	193	29.661	100.743	48.643	1.00	89.37	B	N
ATOM	3344	NH2	ARG	B	193	29.403	98.767	49.786	1.00	90.32	B	N
ATOM	3345	C	ARG	B	193	27.387	98.562	41.562	1.00	69.70	B	C
ATOM	3346	O	ARG	B	193	26.686	99.554	41.366	1.00	70.47	B	O
ATOM	3347	N	ASP	B	194	28.048	97.941	40.588	1.00	33.06	B	N
ATOM	3348	CA	ASP	B	194	27.959	98.408	39.208	1.00	31.59	B	C

ATOM	3349	CB	ASP	B	194	28.840	99.638	38.994	1.00	95.44	B	C
ATOM	3350	CG	ASP	B	194	28.543	100.343	37.682	1.00	96.62	B	C
ATOM	3351	OD1	ASP	B	194	27.448	100.929	37.551	1.00	97.29	B	O
ATOM	3352	OD2	ASP	B	194	29.404	100.304	36.779	1.00	98.87	B	O
ATOM	3353	C	ASP	B	194	28.315	97.356	38.169	1.00	29.95	B	C
ATOM	3354	O	ASP	B	194	29.319	97.467	37.467	1.00	28.49	B	O
ATOM	3355	N	VAL	B	195	27.485	96.325	38.081	1.00	48.93	B	N
ATOM	3356	CA	VAL	B	195	27.695	95.282	37.100	1.00	48.96	B	C
ATOM	3357	CB	VAL	B	195	27.294	93.909	37.622	1.00	31.09	B	C
ATOM	3358	CG1	VAL	B	195	27.280	92.915	36.470	1.00	31.87	B	C
ATOM	3359	CG2	VAL	B	195	28.266	93.470	38.684	1.00	30.66	B	C
ATOM	3360	C	VAL	B	195	26.813	95.616	35.920	1.00	48.14	B	C
ATOM	3361	O	VAL	B	195	25.680	96.049	36.091	1.00	48.59	B	O
ATOM	3362	N	LYS	B	196	27.352	95.417	34.727	1.00	34.77	B	N
ATOM	3363	CA	LYS	B	196	26.648	95.690	33.488	1.00	34.94	B	C
ATOM	3364	CB	LYS	B	196	26.207	97.153	33.430	1.00	62.60	B	C
ATOM	3365	CG	LYS	B	196	27.316	98.170	33.672	1.00	64.55	B	C
ATOM	3366	CD	LYS	B	196	26.741	99.577	33.650	1.00	67.91	B	C
ATOM	3367	CE	LYS	B	196	27.668	100.576	34.305	1.00	70.98	B	C
ATOM	3368	NZ	LYS	B	196	26.968	101.862	34.576	1.00	72.02	B	N
ATOM	3369	C	LYS	B	196	27.612	95.403	32.354	1.00	34.43	B	C
ATOM	3370	O	LYS	B	196	28.816	95.284	32.564	1.00	35.21	B	O
ATOM	3371	N	PRO	B	197	27.105	95.313	31.127	1.00	36.31	B	N
ATOM	3372	CD	PRO	B	197	25.709	95.249	30.675	1.00	27.08	B	C
ATOM	3373	CA	PRO	B	197	28.022	95.027	30.027	1.00	36.33	B	C
ATOM	3374	CB	PRO	B	197	27.097	95.008	28.815	1.00	27.99	B	C
ATOM	3375	CG	PRO	B	197	25.840	94.453	29.387	1.00	27.47	B	C
ATOM	3376	C	PRO	B	197	29.209	95.970	29.862	1.00	37.20	B	C
ATOM	3377	O	PRO	B	197	30.265	95.554	29.395	1.00	35.89	B	O
ATOM	3378	N	SER	B	198	29.044	97.229	30.246	1.00	45.24	B	N
ATOM	3379	CA	SER	B	198	30.124	98.202	30.112	1.00	44.83	B	C
ATOM	3380	CB	SER	B	198	29.549	99.621	30.075	1.00	116.74	B	C
ATOM	3381	OG	SER	B	198	28.683	99.857	31.172	1.00	116.52	B	O
ATOM	3382	C	SER	B	198	31.188	98.118	31.206	1.00	46.38	B	C
ATOM	3383	O	SER	B	198	32.192	98.826	31.168	1.00	46.60	B	O
ATOM	3384	N	ASN	B	199	30.984	97.243	32.177	1.00	38.63	B	N
ATOM	3385	CA	ASN	B	199	31.944	97.131	33.260	1.00	40.21	B	C
ATOM	3386	CB	ASN	B	199	31.252	97.450	34.588	1.00	31.87	B	C
ATOM	3387	CG	ASN	B	199	31.570	98.839	35.089	1.00	34.22	B	C
ATOM	3388	OD1	ASN	B	199	31.733	99.771	34.311	1.00	37.35	B	O
ATOM	3389	ND2	ASN	B	199	31.649	98.983	36.398	1.00	36.18	B	N
ATOM	3390	C	ASN	B	199	32.637	95.778	33.320	1.00	40.72	B	C
ATOM	3391	O	ASN	B	199	33.202	95.404	34.339	1.00	40.47	B	O

ATOM	3392	N	ILE	B	200	32.577	95.040	32.222	1.00	47.09	B	N
ATOM	3393	CA	ILE	B	200	33.248	93.754	32.135	1.00	47.75	B	C
ATOM	3394	CB	ILE	B	200	32.262	92.593	31.907	1.00	41.93	B	C
ATOM	3395	CG2	ILE	B	200	33.016	91.273	31.786	1.00	43.17	B	C
ATOM	3396	CG1	ILE	B	200	31.290	92.502	33.075	1.00	39.80	B	C
ATOM	3397	CD1	ILE	B	200	30.229	91.463	32.859	1.00	36.58	B	C
ATOM	3398	C	ILE	B	200	34.177	93.854	30.933	1.00	50.78	B	C
ATOM	3399	O	ILE	B	200	33.725	93.867	29.790	1.00	51.33	B	O
ATOM	3400	N	LEU	B	201	35.475	93.938	31.197	1.00	40.58	B	N
ATOM	3401	CA	LEU	B	201	36.454	94.047	30.130	1.00	43.98	B	C
ATOM	3402	CB	LEU	B	201	37.538	95.023	30.544	1.00	32.97	B	C
ATOM	3403	CG	LEU	B	201	36.895	96.153	31.338	1.00	32.70	B	C
ATOM	3404	CD1	LEU	B	201	37.902	97.281	31.587	1.00	29.98	B	C
ATOM	3405	CD2	LEU	B	201	35.686	96.645	30.560	1.00	33.92	B	C
ATOM	3406	C	LEU	B	201	37.069	92.702	29.751	1.00	46.61	B	C
ATOM	3407	O	LEU	B	201	37.159	91.786	30.568	1.00	47.21	B	O
ATOM	3408	N	VAL	B	202	37.501	92.600	28.499	1.00	42.60	B	N
ATOM	3409	CA	VAL	B	202	38.082	91.371	27.976	1.00	46.45	B	C
ATOM	3410	CB	VAL	B	202	37.052	90.669	27.107	1.00	19.28	B	C
ATOM	3411	CG1	VAL	B	202	35.753	90.495	27.896	1.00	20.80	B	C
ATOM	3412	CG2	VAL	B	202	36.798	91.496	25.864	1.00	20.29	B	C
ATOM	3413	C	VAL	B	202	39.342	91.646	27.148	1.00	49.17	B	C
ATOM	3414	O	VAL	B	202	39.812	92.781	27.089	1.00	49.29	B	O
ATOM	3415	N	ASN	B	203	39.898	90.610	26.521	1.00	59.31	B	N
ATOM	3416	CA	ASN	B	203	41.103	90.804	25.707	1.00	60.87	B	C
ATOM	3417	CB	ASN	B	203	42.261	91.325	26.566	1.00	48.04	B	C
ATOM	3418	CG	ASN	B	203	42.661	90.363	27.656	1.00	49.60	B	C
ATOM	3419	OD1	ASN	B	203	42.403	89.163	27.565	1.00	50.91	B	O
ATOM	3420	ND2	ASN	B	203	43.311	90.884	28.693	1.00	50.23	B	N
ATOM	3421	C	ASN	B	203	41.622	89.632	24.874	1.00	61.26	B	C
ATOM	3422	O	ASN	B	203	40.991	88.581	24.777	1.00	61.14	B	O
ATOM	3423	N	SER	B	204	42.789	89.858	24.270	1.00	64.59	B	N
ATOM	3424	CA	SER	B	204	43.466	88.891	23.410	1.00	64.02	B	C
ATOM	3425	CB	SER	B	204	44.968	89.194	23.364	1.00	97.55	B	C
ATOM	3426	OG	SER	B	204	45.236	90.386	22.647	1.00	97.23	B	O
ATOM	3427	C	SER	B	204	43.261	87.446	23.832	1.00	63.54	B	C
ATOM	3428	O	SER	B	204	42.795	86.617	23.049	1.00	64.12	B	O
ATOM	3429	N	ARG	B	205	43.638	87.145	25.068	1.00	85.38	B	N
ATOM	3430	CA	ARG	B	205	43.481	85.804	25.602	1.00	85.87	B	C
ATOM	3431	CB	ARG	B	205	44.422	85.609	26.788	1.00	175.80	B	C
ATOM	3432	CG	ARG	B	205	45.800	86.194	26.522	1.00	179.98	B	C
ATOM	3433	CD	ARG	B	205	46.918	85.341	27.097	1.00	183.34	B	C
ATOM	3434	NE	ARG	B	205	48.231	85.919	26.813	1.00	186.61	B	N

ATOM	3435	CZ	ARG	B	205	49.389	85.355	27.145	1.00189.11	B	C
ATOM	3436	NH1	ARG	B	205	50.532	85.958	26.846	1.00190.24	B	N
ATOM	3437	NH2	ARG	B	205	49.406	84.189	27.774	1.00189.87	B	N
ATOM	3438	C	ARG	B	205	42.027	85.696	26.027	1.00 84.32	B	C
ATOM	3439	O	ARG	B	205	41.308	86.692	26.031	1.00 83.74	B	O
ATOM	3440	N	GLY	B	206	41.573	84.502	26.374	1.00 71.98	B	N
ATOM	3441	CA	GLY	B	206	40.183	84.382	26.765	1.00 69.30	B	C
ATOM	3442	C	GLY	B	206	39.879	85.091	28.070	1.00 68.13	B	C
ATOM	3443	O	GLY	B	206	38.980	84.675	28.794	1.00 66.99	B	O
ATOM	3444	N	GLU	B	207	40.605	86.168	28.363	1.00 66.25	B	N
ATOM	3445	CA	GLU	B	207	40.426	86.897	29.613	1.00 63.92	B	C
ATOM	3446	CB	GLU	B	207	41.696	87.667	29.947	1.00 43.77	B	C
ATOM	3447	CG	GLU	B	207	42.852	86.727	30.157	1.00 45.57	B	C
ATOM	3448	CD	GLU	B	207	43.983	87.327	30.946	1.00 46.37	B	C
ATOM	3449	OE1	GLU	B	207	44.776	86.544	31.513	1.00 46.61	B	O
ATOM	3450	OE2	GLU	B	207	44.086	88.569	30.997	1.00 46.35	B	O
ATOM	3451	C	GLU	B	207	39.221	87.813	29.736	1.00 62.77	B	C
ATOM	3452	O	GLU	B	207	38.944	88.647	28.870	1.00 63.40	B	O
ATOM	3453	N	ILE	B	208	38.513	87.632	30.846	1.00 46.59	B	N
ATOM	3454	CA	ILE	B	208	37.319	88.385	31.183	1.00 45.08	B	C
ATOM	3455	CB	ILE	B	208	36.104	87.478	31.161	1.00 28.80	B	C
ATOM	3456	CG2	ILE	B	208	34.936	88.178	31.816	1.00 26.95	B	C
ATOM	3457	CG1	ILE	B	208	35.795	87.048	29.732	1.00 29.50	B	C
ATOM	3458	CD1	ILE	B	208	34.622	86.102	29.656	1.00 29.21	B	C
ATOM	3459	C	ILE	B	208	37.506	88.885	32.606	1.00 44.72	B	C
ATOM	3460	O	ILE	B	208	37.951	88.135	33.464	1.00 44.71	B	O
ATOM	3461	N	LYS	B	209	37.168	90.138	32.873	1.00 32.16	B	N
ATOM	3462	CA	LYS	B	209	37.344	90.663	34.223	1.00 31.40	B	C
ATOM	3463	CB	LYS	B	209	38.721	91.327	34.331	1.00 49.55	B	C
ATOM	3464	CG	LYS	B	209	39.862	90.382	33.970	1.00 51.24	B	C
ATOM	3465	CD	LYS	B	209	41.234	90.987	34.226	1.00 55.73	B	C
ATOM	3466	CE	LYS	B	209	42.329	89.958	33.955	1.00 58.96	B	C
ATOM	3467	NZ	LYS	B	209	43.698	90.530	34.064	1.00 62.07	B	N
ATOM	3468	C	LYS	B	209	36.248	91.644	34.628	1.00 30.45	B	C
ATOM	3469	O	LYS	B	209	35.508	92.124	33.786	1.00 30.55	B	O
ATOM	3470	N	LEU	B	210	36.113	91.907	35.921	1.00 27.34	B	N
ATOM	3471	CA	LEU	B	210	35.120	92.864	36.374	1.00 25.10	B	C
ATOM	3472	CB	LEU	B	210	34.702	92.624	37.816	1.00 19.32	B	C
ATOM	3473	CG	LEU	B	210	33.842	91.381	37.985	1.00 19.23	B	C
ATOM	3474	CD1	LEU	B	210	33.198	91.402	39.346	1.00 18.26	B	C
ATOM	3475	CD2	LEU	B	210	32.796	91.326	36.880	1.00 18.94	B	C
ATOM	3476	C	LEU	B	210	35.811	94.190	36.282	1.00 24.95	B	C
ATOM	3477	O	LEU	B	210	37.016	94.229	36.052	1.00 26.13	B	O

ATOM	3478	N	CYS	B	211	35.058	95.273	36.467	1.00	68.11	B	N
ATOM	3479	CA	CYS	B	211	35.627	96.613	36.385	1.00	67.10	B	C
ATOM	3480	CB	CYS	B	211	35.678	97.061	34.930	1.00	72.82	B	C
ATOM	3481	SG	CYS	B	211	36.661	98.529	34.700	1.00	81.19	B	S
ATOM	3482	C	CYS	B	211	34.838	97.633	37.199	1.00	65.21	B	C
ATOM	3483	O	CYS	B	211	33.733	97.354	37.635	1.00	64.99	B	O
ATOM	3484	N	ASP	B	212	35.426	98.812	37.394	1.00	79.65	B	N
ATOM	3485	CA	ASP	B	212	34.816	99.915	38.146	1.00	79.46	B	C
ATOM	3486	CB	ASP	B	212	33.975	100.796	37.219	1.00	56.99	B	C
ATOM	3487	CG	ASP	B	212	34.792	101.418	36.121	1.00	61.85	B	C
ATOM	3488	OD1	ASP	B	212	35.905	101.898	36.418	1.00	65.25	B	O
ATOM	3489	OD2	ASP	B	212	34.321	101.434	34.964	1.00	60.47	B	O
ATOM	3490	C	ASP	B	212	33.971	99.559	39.358	1.00	79.23	B	C
ATOM	3491	O	ASP	B	212	32.778	99.309	39.241	1.00	78.89	B	O
ATOM	3492	N	PHE	B	213	34.594	99.556	40.528	1.00	31.93	B	N
ATOM	3493	CA	PHE	B	213	33.878	99.269	41.761	1.00	33.23	B	C
ATOM	3494	CB	PHE	B	213	34.050	97.797	42.172	1.00	34.40	B	C
ATOM	3495	CG	PHE	B	213	35.436	97.291	42.019	1.00	32.61	B	C
ATOM	3496	CD1	PHE	B	213	36.315	97.327	43.083	1.00	31.29	B	C
ATOM	3497	CD2	PHE	B	213	35.892	96.854	40.789	1.00	31.55	B	C
ATOM	3498	CE1	PHE	B	213	37.621	96.945	42.917	1.00	31.18	B	C
ATOM	3499	CE2	PHE	B	213	37.199	96.471	40.616	1.00	31.66	B	C
ATOM	3500	CZ	PHE	B	213	38.067	96.517	41.675	1.00	32.43	B	C
ATOM	3501	C	PHE	B	213	34.292	100.233	42.880	1.00	35.36	B	C
ATOM	3502	O	PHE	B	213	35.392	100.795	42.873	1.00	38.18	B	O
ATOM	3503	N	GLY	B	214	33.381	100.425	43.828	1.00	55.99	B	N
ATOM	3504	CA	GLY	B	214	33.608	101.360	44.910	1.00	59.86	B	C
ATOM	3505	C	GLY	B	214	34.592	100.999	45.986	1.00	62.25	B	C
ATOM	3506	O	GLY	B	214	34.206	100.869	47.144	1.00	64.52	B	O
ATOM	3507	N	VAL	B	215	35.861	100.840	45.639	1.00	48.79	B	N
ATOM	3508	CA	VAL	B	215	36.819	100.511	46.680	1.00	50.87	B	C
ATOM	3509	CB	VAL	B	215	38.278	100.325	46.136	1.00	45.25	B	C
ATOM	3510	CG1	VAL	B	215	38.323	99.195	45.123	1.00	45.27	B	C
ATOM	3511	CG2	VAL	B	215	38.796	101.612	45.541	1.00	46.03	B	C
ATOM	3512	C	VAL	B	215	36.774	101.694	47.633	1.00	52.86	B	C
ATOM	3513	O	VAL	B	215	36.749	101.534	48.861	1.00	53.12	B	O
ATOM	3514	N	SER	B	216	36.718	102.878	47.029	1.00	58.08	B	N
ATOM	3515	CA	SER	B	216	36.683	104.157	47.727	1.00	61.13	B	C
ATOM	3516	CB	SER	B	216	37.161	105.267	46.793	1.00	30.78	B	C
ATOM	3517	OG	SER	B	216	36.845	106.539	47.320	1.00	31.78	B	O
ATOM	3518	C	SER	B	216	35.301	104.515	48.222	1.00	62.31	B	C
ATOM	3519	O	SER	B	216	34.319	104.368	47.498	1.00	62.08	B	O
ATOM	3520	N	GLY	B	217	35.233	104.997	49.457	1.00	66.37	B	N

ATOM	3521	CA	GLY	B	217	33.961	105.400	50.023	1.00 67.95	B	C
ATOM	3522	C	GLY	B	217	33.717	106.824	49.581	1.00 68.40	B	C
ATOM	3523	O	GLY	B	217	32.702	107.122	48.953	1.00 68.29	B	O
ATOM	3524	N	GLN	B	218	34.657	107.706	49.909	1.00 82.57	B	N
ATOM	3525	CA	GLN	B	218	34.552	109.101	49.514	1.00 84.79	B	C
ATOM	3526	CB	GLN	B	218	35.859	109.849	49.775	1.00 96.19	B	C
ATOM	3527	CG	GLN	B	218	35.902	111.236	49.149	1.00 96.52	B	C
ATOM	3528	CD	GLN	B	218	34.945	112.216	49.803	1.00 97.82	B	C
ATOM	3529	OE1	GLN	B	218	34.681	113.288	49.263	1.00 99.92	B	O
ATOM	3530	NE2	GLN	B	218	34.429	111.857	50.975	1.00 97.19	B	N
ATOM	3531	C	GLN	B	218	34.255	109.112	48.029	1.00 85.70	B	C
ATOM	3532	O	GLN	B	218	33.133	109.409	47.630	1.00 85.42	B	O
ATOM	3533	N	LEU	B	219	35.253	108.786	47.208	1.00 49.14	B	N
ATOM	3534	CA	LEU	B	219	35.027	108.755	45.768	1.00 49.20	B	C
ATOM	3535	CB	LEU	B	219	36.270	108.324	45.002	1.00112.27	B	C
ATOM	3536	CG	LEU	B	219	36.070	108.517	43.495	1.00111.82	B	C
ATOM	3537	CD1	LEU	B	219	35.103	107.488	42.935	1.00110.11	B	C
ATOM	3538	CD2	LEU	B	219	35.548	109.923	43.252	1.00111.82	B	C
ATOM	3539	C	LEU	B	219	33.917	107.755	45.539	1.00 52.39	B	C
ATOM	3540	O	LEU	B	219	34.089	106.552	45.730	1.00 52.05	B	O
ATOM	3541	N	ILE	B	220	32.786	108.287	45.105	1.00 76.50	B	N
ATOM	3542	CA	ILE	B	220	31.558	107.542	44.874	1.00 75.79	B	C
ATOM	3543	CB	ILE	B	220	31.367	106.398	45.922	1.00 75.74	B	C
ATOM	3544	CG2	ILE	B	220	29.938	106.390	46.442	1.00 76.75	B	C
ATOM	3545	CG1	ILE	B	220	31.727	105.039	45.311	1.00 76.05	B	C
ATOM	3546	CD1	ILE	B	220	31.546	103.870	46.271	1.00 75.34	B	C
ATOM	3547	C	ILE	B	220	30.566	108.649	45.185	1.00 77.82	B	C
ATOM	3548	O	ILE	B	220	29.495	108.758	44.581	1.00 78.76	B	O
ATOM	3549	N	ASP	B	221	30.980	109.480	46.142	1.00157.52	B	N
ATOM	3550	CA	ASP	B	221	30.208	110.617	46.622	1.00159.07	B	C
ATOM	3551	CB	ASP	B	221	30.129	110.610	48.148	1.00 92.31	B	C
ATOM	3552	CG	ASP	B	221	29.554	109.325	48.695	1.00 92.16	B	C
ATOM	3553	OD1	ASP	B	221	30.278	108.308	48.717	1.00 92.62	B	O
ATOM	3554	OD2	ASP	B	221	28.372	109.326	49.093	1.00 91.93	B	O
ATOM	3555	C	ASP	B	221	30.796	111.943	46.173	1.00161.64	B	C
ATOM	3556	O	ASP	B	221	30.118	112.970	46.244	1.00161.95	B	O
ATOM	3557	N	SER	B	222	32.053	111.939	45.734	1.00167.80	B	N
ATOM	3558	CA	SER	B	222	32.645	113.184	45.268	1.00169.22	B	C
ATOM	3559	CB	SER	B	222	34.012	112.951	44.617	1.00 87.83	B	C
ATOM	3560	OG	SER	B	222	34.640	114.189	44.319	1.00 86.59	B	O
ATOM	3561	C	SER	B	222	31.618	113.627	44.244	1.00170.52	B	C
ATOM	3562	O	SER	B	222	31.383	114.822	44.048	1.00171.02	B	O
ATOM	3563	N	MET	B	223	30.995	112.626	43.617	1.00149.31	B	N

ATOM	3564	CA	MET	B	223	29.929	112.824	42.643	1.00149.54	B	C
ATOM	3565	CB	MET	B	223	30.015	111.812	41.493	1.00156.64	B	C
ATOM	3566	CG	MET	B	223	31.249	111.960	40.614	1.00155.25	B	C
ATOM	3567	SD	MET	B	223	31.207	110.920	39.135	1.00154.91	B	S
ATOM	3568	CE	MET	B	223	32.012	109.415	39.742	1.00154.30	B	C
ATOM	3569	C	MET	B	223	28.662	112.571	43.443	1.00149.75	B	C
ATOM	3570	O	MET	B	223	27.807	113.447	43.548	1.00152.72	B	O
ATOM	3571	N	ALA	B	224	28.572	111.375	44.021	1.00112.40	B	N
ATOM	3572	CA	ALA	B	224	27.444	110.956	44.847	1.00112.61	B	C
ATOM	3573	CB	ALA	B	224	27.060	112.050	45.843	1.00116.84	B	C
ATOM	3574	C	ALA	B	224	26.232	110.560	44.053	1.00112.31	B	C
ATOM	3575	O	ALA	B	224	25.890	109.382	44.013	1.00112.04	B	O
ATOM	3576	N	ASN	B	225	25.586	111.558	43.445	1.00198.83	B	N
ATOM	3577	CA	ASN	B	225	24.375	111.355	42.660	1.00198.98	B	C
ATOM	3578	CB	ASN	B	225	23.992	112.647	41.975	1.00176.84	B	C
ATOM	3579	CG	ASN	B	225	23.706	113.723	42.984	1.00177.11	B	C
ATOM	3580	OD1	ASN	B	225	22.650	113.731	43.625	1.00176.85	B	O
ATOM	3581	ND2	ASN	B	225	24.672	114.604	43.189	1.00177.26	B	N
ATOM	3582	C	ASN	B	225	24.623	110.239	41.721	1.00199.67	B	C
ATOM	3583	O	ASN	B	225	24.722	110.367	40.488	1.00199.92	B	O
ATOM	3584	N	SER	B	226	24.741	109.091	42.358	1.00203.67	B	N
ATOM	3585	CA	SER	B	226	25.001	107.940	41.579	1.00203.67	B	C
ATOM	3586	CB	SER	B	226	25.444	106.727	42.408	1.00203.67	B	C
ATOM	3587	OG	SER	B	226	26.652	106.259	41.821	1.00203.67	B	O
ATOM	3588	C	SER	B	226	23.756	107.629	40.795	1.00203.67	B	C
ATOM	3589	O	SER	B	226	22.653	107.734	41.289	1.00203.67	B	O
ATOM	3590	N	PHE	B	227	24.026	107.415	39.514	1.00203.67	B	N
ATOM	3591	CA	PHE	B	227	23.145	106.912	38.460	1.00203.67	B	C
ATOM	3592	CB	PHE	B	227	22.502	105.633	38.985	1.00203.67	B	C
ATOM	3593	CG	PHE	B	227	23.433	104.511	39.056	1.00203.67	B	C
ATOM	3594	CD1	PHE	B	227	24.110	104.225	40.230	1.00203.67	B	C
ATOM	3595	CD2	PHE	B	227	23.674	103.779	37.913	1.00203.67	B	C
ATOM	3596	CE1	PHE	B	227	25.013	103.214	40.241	1.00203.67	B	C
ATOM	3597	CE2	PHE	B	227	24.553	102.798	37.922	1.00203.67	B	C
ATOM	3598	CZ	PHE	B	227	25.228	102.500	39.069	1.00203.67	B	C
ATOM	3599	C	PHE	B	227	22.225	107.441	37.442	1.00203.67	B	C
ATOM	3600	O	PHE	B	227	21.753	108.552	37.416	1.00203.67	B	O
ATOM	3601	N	VAL	B	228	22.221	106.474	36.452	1.00176.22	B	N
ATOM	3602	CA	VAL	B	228	21.466	106.274	35.241	1.00175.44	B	C
ATOM	3603	CB	VAL	B	228	20.195	105.346	35.680	1.00125.13	B	C
ATOM	3604	CG1	VAL	B	228	19.104	106.266	36.402	1.00125.42	B	C
ATOM	3605	CG2	VAL	B	228	19.629	104.579	34.505	1.00125.06	B	C
ATOM	3606	C	VAL	B	228	20.926	107.366	34.246	1.00174.58	B	C

ATOM	3607	O	VAL	B	228	21.533	108.445	33.935	1.00174.73	B	O
ATOM	3608	N	GLY	B	229	19.783	107.015	33.762	1.00146.34	B	N
ATOM	3609	CA	GLY	B	229	19.095	107.849	32.808	1.00144.37	B	C
ATOM	3610	C	GLY	B	229	19.005	106.836	31.695	1.00143.27	B	C
ATOM	3611	O	GLY	B	229	17.894	106.393	31.503	1.00142.89	B	O
ATOM	3612	N	THR	B	230	20.066	106.451	30.965	1.00200.92	B	N
ATOM	3613	CA	THR	B	230	19.859	105.365	29.945	1.00199.70	B	C
ATOM	3614	CB	THR	B	230	20.862	105.393	28.700	1.00178.33	B	C
ATOM	3615	OG1	THR	B	230	20.303	104.626	27.607	1.00180.07	B	O
ATOM	3616	CG2	THR	B	230	22.207	104.751	29.063	1.00177.92	B	C
ATOM	3617	C	THR	B	230	19.905	103.903	30.526	1.00197.85	B	C
ATOM	3618	O	THR	B	230	20.877	103.486	31.176	1.00196.84	B	O
ATOM	3619	N	ARG	B	231	18.860	103.121	30.254	1.00 72.55	B	N
ATOM	3620	CA	ARG	B	231	18.757	101.728	30.719	1.00 68.93	B	C
ATOM	3621	CB	ARG	B	231	19.944	100.917	30.173	1.00203.67	B	C
ATOM	3622	CG	ARG	B	231	20.142	101.127	28.668	1.00203.67	B	C
ATOM	3623	CD	ARG	B	231	18.833	100.897	27.908	1.00203.67	B	C
ATOM	3624	NE	ARG	B	231	18.823	99.619	27.200	1.00203.67	B	N
ATOM	3625	CZ	ARG	B	231	19.094	99.488	25.909	1.00203.67	B	C
ATOM	3626	NH1	ARG	B	231	19.386	100.568	25.189	1.00203.67	B	N
ATOM	3627	NH2	ARG	B	231	19.105	98.287	25.338	1.00203.67	B	N
ATOM	3628	C	ARG	B	231	18.667	101.650	32.251	1.00 66.21	B	C
ATOM	3629	O	ARG	B	231	17.718	102.169	32.820	1.00 66.36	B	O
ATOM	3630	N	SER	B	232	19.646	101.023	32.900	1.00 38.12	B	N
ATOM	3631	CA	SER	B	232	19.739	100.849	34.375	1.00 34.16	B	C
ATOM	3632	CB	SER	B	232	18.510	101.352	35.125	1.00 53.49	B	C
ATOM	3633	OG	SER	B	232	18.619	101.014	36.496	1.00 52.48	B	O
ATOM	3634	C	SER	B	232	19.917	99.383	34.740	1.00 30.96	B	C
ATOM	3635	O	SER	B	232	19.209	98.534	34.228	1.00 31.04	B	O
ATOM	3636	N	TYR	B	233	20.831	99.095	35.649	1.00 66.68	B	N
ATOM	3637	CA	TYR	B	233	21.097	97.709	36.021	1.00 62.81	B	C
ATOM	3638	CB	TYR	B	233	22.478	97.337	35.531	1.00 35.15	B	C
ATOM	3639	CG	TYR	B	233	22.564	97.337	34.043	1.00 30.23	B	C
ATOM	3640	CD1	TYR	B	233	22.052	96.276	33.310	1.00 30.11	B	C
ATOM	3641	CE1	TYR	B	233	22.113	96.260	31.939	1.00 29.50	B	C
ATOM	3642	CD2	TYR	B	233	23.140	98.391	33.365	1.00 27.87	B	C
ATOM	3643	CE2	TYR	B	233	23.207	98.390	32.000	1.00 27.56	B	C
ATOM	3644	CZ	TYR	B	233	22.692	97.316	31.284	1.00 28.17	B	C
ATOM	3645	OH	TYR	B	233	22.764	97.289	29.908	1.00 26.88	B	O
ATOM	3646	C	TYR	B	233	21.011	97.474	37.508	1.00 63.29	B	C
ATOM	3647	O	TYR	B	233	21.419	96.428	38.021	1.00 64.68	B	O
ATOM	3648	N	MET	B	234	20.474	98.471	38.192	1.00 41.61	B	N
ATOM	3649	CA	MET	B	234	20.323	98.436	39.624	1.00 40.29	B	C

ATOM	3650	CB	MET	B	234	20.159	99.847	40.132	1.00	54.77	B	C
ATOM	3651	CG	MET	B	234	19.922	99.922	41.588	1.00	57.11	B	C
ATOM	3652	SD	MET	B	234	20.256	101.580	42.028	1.00	59.47	B	S
ATOM	3653	CE	MET	B	234	21.744	101.889	41.003	1.00	58.55	B	C
ATOM	3654	C	MET	B	234	19.134	97.609	40.032	1.00	39.32	B	C
ATOM	3655	O	MET	B	234	18.070	97.692	39.430	1.00	38.70	B	O
ATOM	3656	N	ALA	B	235	19.327	96.816	41.075	1.00	35.39	B	N
ATOM	3657	CA	ALA	B	235	18.275	95.953	41.588	1.00	36.56	B	C
ATOM	3658	CB	ALA	B	235	18.868	94.942	42.564	1.00	121.70	B	C
ATOM	3659	C	ALA	B	235	17.144	96.720	42.260	1.00	37.42	B	C
ATOM	3660	O	ALA	B	235	17.326	97.831	42.758	1.00	38.21	B	O
ATOM	3661	N	PRO	B	236	15.950	96.127	42.274	1.00	41.47	B	N
ATOM	3662	CD	PRO	B	236	15.588	94.831	41.675	1.00	34.73	B	C
ATOM	3663	CA	PRO	B	236	14.790	96.760	42.893	1.00	42.53	B	C
ATOM	3664	CB	PRO	B	236	13.785	95.614	42.958	1.00	33.87	B	C
ATOM	3665	CG	PRO	B	236	14.074	94.873	41.697	1.00	34.57	B	C
ATOM	3666	C	PRO	B	236	15.123	97.324	44.273	1.00	44.17	B	C
ATOM	3667	O	PRO	B	236	15.013	98.521	44.510	1.00	44.62	B	O
ATOM	3668	N	GLU	B	237	15.551	96.448	45.173	1.00	39.53	B	N
ATOM	3669	CA	GLU	B	237	15.874	96.844	46.535	1.00	40.79	B	C
ATOM	3670	CB	GLU	B	237	16.477	95.686	47.329	1.00	48.23	B	C
ATOM	3671	CG	GLU	B	237	17.921	95.416	47.000	1.00	47.09	B	C
ATOM	3672	CD	GLU	B	237	18.081	94.251	46.063	1.00	46.32	B	C
ATOM	3673	OE1	GLU	B	237	17.320	94.180	45.080	1.00	46.23	B	O
ATOM	3674	OE2	GLU	B	237	18.970	93.408	46.306	1.00	44.71	B	O
ATOM	3675	C	GLU	B	237	16.836	97.993	46.605	1.00	42.05	B	C
ATOM	3676	O	GLU	B	237	16.917	98.663	47.616	1.00	43.50	B	O
ATOM	3677	N	ARG	B	238	17.588	98.228	45.550	1.00	16.39	B	N
ATOM	3678	CA	ARG	B	238	18.521	99.329	45.612	1.00	19.76	B	C
ATOM	3679	CB	ARG	B	238	19.738	99.044	44.729	1.00	24.18	B	C
ATOM	3680	CG	ARG	B	238	21.031	99.646	45.247	1.00	29.27	B	C
ATOM	3681	CD	ARG	B	238	22.180	99.394	44.307	1.00	34.12	B	C
ATOM	3682	NE	ARG	B	238	23.349	100.168	44.699	1.00	39.45	B	N
ATOM	3683	CZ	ARG	B	238	24.373	100.450	43.900	1.00	41.53	B	C
ATOM	3684	NH1	ARG	B	238	24.401	100.028	42.642	1.00	42.34	B	N
ATOM	3685	NH2	ARG	B	238	25.376	101.173	44.363	1.00	43.23	B	N
ATOM	3686	C	ARG	B	238	17.818	100.613	45.177	1.00	20.88	B	C
ATOM	3687	O	ARG	B	238	18.362	101.704	45.305	1.00	21.31	B	O
ATOM	3688	N	LEU	B	239	16.595	100.472	44.678	1.00	46.46	B	N
ATOM	3689	CA	LEU	B	239	15.817	101.617	44.227	1.00	47.50	B	C
ATOM	3690	CB	LEU	B	239	15.369	101.439	42.780	1.00	19.24	B	C
ATOM	3691	CG	LEU	B	239	16.318	100.947	41.694	1.00	16.92	B	C
ATOM	3692	CD1	LEU	B	239	15.465	100.431	40.540	1.00	13.37	B	C

ATOM	3693	CD2	LEU	B	239	17.252	102.032	41.240	1.00 15.22	B	C
ATOM	3694	C	LEU	B	239	14.564	101.767	45.067	1.00 49.79	B	C
ATOM	3695	O	LEU	B	239	13.520	102.118	44.540	1.00 48.63	B	O
ATOM	3696	N	GLN	B	240	14.634	101.487	46.358	1.00 45.31	B	N
ATOM	3697	CA	GLN	B	240	13.445	101.629	47.179	1.00 49.67	B	C
ATOM	3698	CB	GLN	B	240	12.665	100.324	47.215	1.00 59.80	B	C
ATOM	3699	CG	GLN	B	240	12.343	99.778	45.852	1.00 60.88	B	C
ATOM	3700	CD	GLN	B	240	11.360	98.630	45.901	1.00 62.99	B	C
ATOM	3701	OE1	GLN	B	240	11.088	97.987	44.885	1.00 65.89	B	O
ATOM	3702	NE2	GLN	B	240	10.811	98.371	47.083	1.00 63.64	B	N
ATOM	3703	C	GLN	B	240	13.808	102.031	48.586	1.00 53.12	B	C
ATOM	3704	O	GLN	B	240	13.025	102.686	49.273	1.00 53.65	B	O
ATOM	3705	N	GLY	B	241	15.004	101.638	49.006	1.00 39.31	B	N
ATOM	3706	CA	GLY	B	241	15.473	101.939	50.341	1.00 44.03	B	C
ATOM	3707	C	GLY	B	241	16.956	101.650	50.385	1.00 47.78	B	C
ATOM	3708	O	GLY	B	241	17.575	101.425	49.342	1.00 48.00	B	O
ATOM	3709	N	THR	B	242	17.532	101.642	51.582	1.00161.88	B	N
ATOM	3710	CA	THR	B	242	18.963	101.406	51.738	1.00163.49	B	C
ATOM	3711	CB	THR	B	242	19.576	102.426	52.727	1.00183.33	B	C
ATOM	3712	OG1	THR	B	242	20.998	102.260	52.776	1.00183.20	B	O
ATOM	3713	CG2	THR	B	242	18.997	102.231	54.121	1.00182.11	B	C
ATOM	3714	C	THR	B	242	19.313	99.996	52.207	1.00165.15	B	C
ATOM	3715	O	THR	B	242	20.330	99.793	52.868	1.00167.66	B	O
ATOM	3716	N	HIS	B	243	18.482	99.018	51.863	1.00 89.69	B	N
ATOM	3717	CA	HIS	B	243	18.760	97.648	52.277	1.00 89.77	B	C
ATOM	3718	CB	HIS	B	243	17.481	96.955	52.757	1.00203.67	B	C
ATOM	3719	CG	HIS	B	243	17.208	97.134	54.219	1.00203.67	B	C
ATOM	3720	CD2	HIS	B	243	16.076	97.470	54.882	1.00203.67	B	C
ATOM	3721	ND1	HIS	B	243	18.169	96.927	55.185	1.00203.67	B	N
ATOM	3722	CE1	HIS	B	243	17.642	97.127	56.379	1.00203.67	B	C
ATOM	3723	NE2	HIS	B	243	16.372	97.457	56.223	1.00203.67	B	N
ATOM	3724	C	HIS	B	243	19.417	96.805	51.193	1.00 89.14	B	C
ATOM	3725	O	HIS	B	243	19.057	95.642	51.000	1.00 89.64	B	O
ATOM	3726	N	TYR	B	244	20.382	97.387	50.487	1.00 61.14	B	N
ATOM	3727	CA	TYR	B	244	21.069	96.647	49.443	1.00 59.55	B	C
ATOM	3728	CB	TYR	B	244	21.525	97.582	48.305	1.00122.00	B	C
ATOM	3729	CG	TYR	B	244	22.631	98.565	48.632	1.00125.09	B	C
ATOM	3730	CD1	TYR	B	244	23.928	98.135	48.871	1.00126.93	B	C
ATOM	3731	CE1	TYR	B	244	24.943	99.035	49.147	1.00128.51	B	C
ATOM	3732	CD2	TYR	B	244	22.379	99.930	48.676	1.00125.32	B	C
ATOM	3733	CE2	TYR	B	244	23.386	100.838	48.949	1.00127.02	B	C
ATOM	3734	CZ	TYR	B	244	24.665	100.385	49.185	1.00128.42	B	C
ATOM	3735	OH	TYR	B	244	25.666	101.285	49.472	1.00130.04	B	O

ATOM	3736	C	TYR	B	244	22.246	95.889	50.035	1.00	55.65	B	C
ATOM	3737	O	TYR	B	244	22.944	96.392	50.916	1.00	55.68	B	O
ATOM	3738	N	SER	B	245	22.439	94.659	49.569	1.00	58.50	B	N
ATOM	3739	CA	SER	B	245	23.533	93.822	50.039	1.00	53.69	B	C
ATOM	3740	CB	SER	B	245	22.983	92.555	50.684	1.00	89.45	B	C
ATOM	3741	OG	SER	B	245	24.037	91.766	51.203	1.00	90.88	B	O
ATOM	3742	C	SER	B	245	24.437	93.446	48.873	1.00	50.65	B	C
ATOM	3743	O	SER	B	245	24.854	94.292	48.092	1.00	52.58	B	O
ATOM	3744	N	VAL	B	246	24.741	92.166	48.760	1.00	51.19	B	N
ATOM	3745	CA	VAL	B	246	25.581	91.695	47.680	1.00	47.92	B	C
ATOM	3746	CB	VAL	B	246	26.648	90.724	48.200	1.00	74.56	B	C
ATOM	3747	CG1	VAL	B	246	27.564	90.276	47.056	1.00	72.81	B	C
ATOM	3748	CG2	VAL	B	246	27.435	91.401	49.317	1.00	74.67	B	C
ATOM	3749	C	VAL	B	246	24.685	90.985	46.692	1.00	44.20	B	C
ATOM	3750	O	VAL	B	246	25.127	90.545	45.644	1.00	43.24	B	O
ATOM	3751	N	GLN	B	247	23.415	90.861	47.036	1.00	46.46	B	N
ATOM	3752	CA	GLN	B	247	22.493	90.205	46.135	1.00	41.48	B	C
ATOM	3753	CB	GLN	B	247	21.219	89.785	46.873	1.00	46.49	B	C
ATOM	3754	CG	GLN	B	247	21.419	88.656	47.886	1.00	49.32	B	C
ATOM	3755	CD	GLN	B	247	22.190	87.469	47.317	1.00	51.40	B	C
ATOM	3756	OE1	GLN	B	247	21.946	87.037	46.189	1.00	53.90	B	O
ATOM	3757	NE2	GLN	B	247	23.120	86.933	48.104	1.00	52.33	B	N
ATOM	3758	C	GLN	B	247	22.167	91.175	45.005	1.00	39.91	B	C
ATOM	3759	O	GLN	B	247	21.837	90.765	43.888	1.00	40.09	B	O
ATOM	3760	N	SER	B	248	22.284	92.468	45.295	1.00	41.90	B	N
ATOM	3761	CA	SER	B	248	22.002	93.479	44.295	1.00	40.15	B	C
ATOM	3762	CB	SER	B	248	22.203	94.864	44.882	1.00	40.73	B	C
ATOM	3763	OG	SER	B	248	23.582	95.159	44.937	1.00	40.03	B	O
ATOM	3764	C	SER	B	248	22.940	93.282	43.103	1.00	38.24	B	C
ATOM	3765	O	SER	B	248	22.637	93.705	41.991	1.00	38.31	B	O
ATOM	3766	N	ASP	B	249	24.080	92.639	43.338	1.00	26.45	B	N
ATOM	3767	CA	ASP	B	249	25.034	92.396	42.268	1.00	24.94	B	C
ATOM	3768	CB	ASP	B	249	26.458	92.215	42.808	1.00	43.77	B	C
ATOM	3769	CG	ASP	B	249	27.126	93.530	43.171	1.00	45.13	B	C
ATOM	3770	OD1	ASP	B	249	26.915	94.531	42.459	1.00	45.87	B	O
ATOM	3771	OD2	ASP	B	249	27.883	93.557	44.159	1.00	46.43	B	O
ATOM	3772	C	ASP	B	249	24.634	91.169	41.469	1.00	23.91	B	C
ATOM	3773	O	ASP	B	249	24.981	91.052	40.292	1.00	24.76	B	O
ATOM	3774	N	ILE	B	250	23.914	90.240	42.089	1.00	40.28	B	N
ATOM	3775	CA	ILE	B	250	23.493	89.069	41.334	1.00	37.47	B	C
ATOM	3776	CB	ILE	B	250	22.773	88.009	42.200	1.00	42.48	B	C
ATOM	3777	CG2	ILE	B	250	22.363	86.845	41.317	1.00	42.60	B	C
ATOM	3778	CG1	ILE	B	250	23.692	87.488	43.321	1.00	42.48	B	C

ATOM	3779	CD1	ILE	B	250	24.829	86.612	42.856	1.00	42.48	B	C
ATOM	3780	C	ILE	B	250	22.516	89.583	40.283	1.00	37.95	B	C
ATOM	3781	O	ILE	B	250	22.603	89.200	39.120	1.00	38.10	B	O
ATOM	3782	N	TRP	B	251	21.604	90.467	40.699	1.00	28.95	B	N
ATOM	3783	CA	TRP	B	251	20.609	91.065	39.793	1.00	28.93	B	C
ATOM	3784	CB	TRP	B	251	19.698	92.058	40.558	1.00	29.90	B	C
ATOM	3785	CG	TRP	B	251	18.800	92.916	39.677	1.00	29.90	B	C
ATOM	3786	CD2	TRP	B	251	17.422	92.680	39.350	1.00	29.90	B	C
ATOM	3787	CE2	TRP	B	251	17.026	93.690	38.441	1.00	30.30	B	C
ATOM	3788	CE3	TRP	B	251	16.485	91.709	39.730	1.00	29.90	B	C
ATOM	3789	CD1	TRP	B	251	19.163	94.034	38.978	1.00	29.90	B	C
ATOM	3790	NE1	TRP	B	251	18.106	94.503	38.233	1.00	29.90	B	N
ATOM	3791	CZ2	TRP	B	251	15.743	93.757	37.908	1.00	30.46	B	C
ATOM	3792	CZ3	TRP	B	251	15.208	91.775	39.198	1.00	30.26	B	C
ATOM	3793	CH2	TRP	B	251	14.849	92.795	38.292	1.00	31.40	B	C
ATOM	3794	C	TRP	B	251	21.309	91.764	38.629	1.00	28.93	B	C
ATOM	3795	O	TRP	B	251	21.088	91.431	37.464	1.00	28.97	B	O
ATOM	3796	N	SER	B	252	22.162	92.727	38.944	1.00	31.12	B	N
ATOM	3797	CA	SER	B	252	22.872	93.439	37.902	1.00	32.38	B	C
ATOM	3798	CB	SER	B	252	24.006	94.274	38.494	1.00	42.77	B	C
ATOM	3799	OG	SER	B	252	23.486	95.337	39.274	1.00	46.97	B	O
ATOM	3800	C	SER	B	252	23.429	92.409	36.947	1.00	32.02	B	C
ATOM	3801	O	SER	B	252	23.238	92.513	35.738	1.00	33.80	B	O
ATOM	3802	N	MET	B	253	24.101	91.398	37.492	1.00	9.88	B	N
ATOM	3803	CA	MET	B	253	24.679	90.365	36.653	1.00	11.08	B	C
ATOM	3804	CB	MET	B	253	25.423	89.340	37.482	1.00	29.48	B	C
ATOM	3805	CG	MET	B	253	25.720	88.077	36.693	1.00	31.23	B	C
ATOM	3806	SD	MET	B	253	25.889	86.664	37.762	1.00	32.78	B	S
ATOM	3807	CE	MET	B	253	27.547	86.927	38.174	1.00	32.81	B	C
ATOM	3808	C	MET	B	253	23.615	89.645	35.872	1.00	10.69	B	C
ATOM	3809	O	MET	B	253	23.785	89.392	34.686	1.00	11.44	B	O
ATOM	3810	N	GLY	B	254	22.523	89.311	36.555	1.00	36.83	B	N
ATOM	3811	CA	GLY	B	254	21.422	88.596	35.934	1.00	36.15	B	C
ATOM	3812	C	GLY	B	254	20.834	89.287	34.721	1.00	36.15	B	C
ATOM	3813	O	GLY	B	254	20.505	88.638	33.729	1.00	36.21	B	O
ATOM	3814	N	LEU	B	255	20.695	90.604	34.798	1.00	23.53	B	N
ATOM	3815	CA	LEU	B	255	20.156	91.368	33.689	1.00	23.53	B	C
ATOM	3816	CB	LEU	B	255	19.820	92.782	34.151	1.00	32.07	B	C
ATOM	3817	CG	LEU	B	255	18.804	93.574	33.328	1.00	31.25	B	C
ATOM	3818	CD1	LEU	B	255	17.401	93.049	33.587	1.00	31.51	B	C
ATOM	3819	CD2	LEU	B	255	18.906	95.023	33.703	1.00	31.62	B	C
ATOM	3820	C	LEU	B	255	21.172	91.434	32.547	1.00	25.76	B	C
ATOM	3821	O	LEU	B	255	20.850	91.121	31.406	1.00	23.53	B	O

ATOM	3822	N	SER	B	256	22.393	91.851	32.868	1.00 36.71	B	N
ATOM	3823	CA	SER	B	256	23.482	91.962	31.900	1.00 36.39	B	C
ATOM	3824	CB	SER	B	256	24.804	92.204	32.642	1.00 27.70	B	C
ATOM	3825	OG	SER	B	256	24.690	93.187	33.656	1.00 28.79	B	O
ATOM	3826	C	SER	B	256	23.620	90.694	31.032	1.00 36.53	B	C
ATOM	3827	O	SER	B	256	23.873	90.771	29.818	1.00 35.75	B	O
ATOM	3828	N	LEU	B	257	23.478	89.528	31.661	1.00 23.61	B	N
ATOM	3829	CA	LEU	B	257	23.575	88.270	30.938	1.00 23.68	B	C
ATOM	3830	CB	LEU	B	257	23.491	87.080	31.905	1.00 14.08	B	C
ATOM	3831	CG	LEU	B	257	24.755	86.282	32.266	1.00 13.54	B	C
ATOM	3832	CD1	LEU	B	257	26.009	87.116	32.040	1.00 13.01	B	C
ATOM	3833	CD2	LEU	B	257	24.635	85.820	33.714	1.00 15.29	B	C
ATOM	3834	C	LEU	B	257	22.441	88.204	29.932	1.00 25.85	B	C
ATOM	3835	O	LEU	B	257	22.664	87.853	28.781	1.00 26.72	B	O
ATOM	3836	N	VAL	B	258	21.230	88.548	30.368	1.00 34.52	B	N
ATOM	3837	CA	VAL	B	258	20.061	88.543	29.490	1.00 34.69	B	C
ATOM	3838	CB	VAL	B	258	18.795	88.913	30.258	1.00 52.73	B	C
ATOM	3839	CG1	VAL	B	258	17.591	88.873	29.340	1.00 53.02	B	C
ATOM	3840	CG2	VAL	B	258	18.606	87.951	31.401	1.00 51.68	B	C
ATOM	3841	C	VAL	B	258	20.224	89.530	28.338	1.00 35.81	B	C
ATOM	3842	O	VAL	B	258	19.761	89.291	27.226	1.00 36.14	B	O
ATOM	3843	N	GLU	B	259	20.881	90.647	28.607	1.00 38.67	B	N
ATOM	3844	CA	GLU	B	259	21.108	91.651	27.584	1.00 37.69	B	C
ATOM	3845	CB	GLU	B	259	21.786	92.869	28.197	1.00 52.24	B	C
ATOM	3846	CG	GLU	B	259	22.162	93.953	27.212	1.00 52.61	B	C
ATOM	3847	CD	GLU	B	259	22.296	95.289	27.896	1.00 51.00	B	C
ATOM	3848	OE1	GLU	B	259	22.667	96.277	27.238	1.00 49.46	B	O
ATOM	3849	OE2	GLU	B	259	22.019	95.344	29.108	1.00 49.86	B	O
ATOM	3850	C	GLU	B	259	21.987	91.068	26.497	1.00 37.97	B	C
ATOM	3851	O	GLU	B	259	21.573	90.970	25.346	1.00 35.98	B	O
ATOM	3852	N	LEU	B	260	23.203	90.679	26.871	1.00 71.01	B	N
ATOM	3853	CA	LEU	B	260	24.158	90.090	25.932	1.00 71.10	B	C
ATOM	3854	CB	LEU	B	260	25.440	89.714	26.678	1.00 37.85	B	C
ATOM	3855	CG	LEU	B	260	26.140	90.842	27.446	1.00 39.29	B	C
ATOM	3856	CD1	LEU	B	260	26.972	90.266	28.569	1.00 39.08	B	C
ATOM	3857	CD2	LEU	B	260	27.016	91.648	26.496	1.00 38.24	B	C
ATOM	3858	C	LEU	B	260	23.562	88.849	25.261	1.00 70.82	B	C
ATOM	3859	O	LEU	B	260	24.029	88.409	24.221	1.00 69.07	B	O
ATOM	3860	N	ALA	B	261	22.520	88.298	25.869	1.00 30.15	B	N
ATOM	3861	CA	ALA	B	261	21.843	87.119	25.358	1.00 30.17	B	C
ATOM	3862	CB	ALA	B	261	21.111	86.424	26.491	1.00 4.67	B	C
ATOM	3863	C	ALA	B	261	20.850	87.481	24.261	1.00 29.14	B	C
ATOM	3864	O	ALA	B	261	20.770	86.809	23.234	1.00 29.98	B	O

ATOM	3865	N	VAL	B	262	20.079	88.538	24.494	1.00	41.21	B	N
ATOM	3866	CA	VAL	B	262	19.081	88.988	23.531	1.00	41.39	B	C
ATOM	3867	CB	VAL	B	262	17.682	89.107	24.165	1.00	26.46	B	C
ATOM	3868	CG1	VAL	B	262	16.628	88.909	23.095	1.00	26.35	B	C
ATOM	3869	CG2	VAL	B	262	17.511	88.127	25.298	1.00	24.48	B	C
ATOM	3870	C	VAL	B	262	19.402	90.364	22.967	1.00	42.96	B	C
ATOM	3871	O	VAL	B	262	18.691	91.312	23.260	1.00	40.83	B	O
ATOM	3872	N	GLY	B	263	20.463	90.477	22.176	1.00	80.74	B	N
ATOM	3873	CA	GLY	B	263	20.834	91.752	21.573	1.00	82.13	B	C
ATOM	3874	C	GLY	B	263	20.818	93.034	22.402	1.00	83.22	B	C
ATOM	3875	O	GLY	B	263	21.827	93.735	22.473	1.00	84.46	B	O
ATOM	3876	N	ARG	B	264	19.686	93.358	23.022	1.00	74.74	B	N
ATOM	3877	CA	ARG	B	264	19.569	94.582	23.820	1.00	75.63	B	C
ATOM	3878	CB	ARG	B	264	18.594	95.541	23.132	1.00	89.01	B	C
ATOM	3879	CG	ARG	B	264	17.480	94.831	22.369	1.00	93.98	B	C
ATOM	3880	CD	ARG	B	264	16.653	93.947	23.281	1.00	97.84	B	C
ATOM	3881	NE	ARG	B	264	15.763	94.734	24.124	1.00	101.55	B	N
ATOM	3882	CZ	ARG	B	264	14.686	95.366	23.674	1.00	104.80	B	C
ATOM	3883	NH1	ARG	B	264	14.369	95.299	22.386	1.00	106.89	B	N
ATOM	3884	NH2	ARG	B	264	13.925	96.061	24.510	1.00	106.81	B	N
ATOM	3885	C	ARG	B	264	19.163	94.417	25.293	1.00	76.04	B	C
ATOM	3886	O	ARG	B	264	19.060	93.302	25.808	1.00	74.80	B	O
ATOM	3887	N	TYR	B	265	18.930	95.554	25.950	1.00	12.23	B	N
ATOM	3888	CA	TYR	B	265	18.543	95.628	27.360	1.00	11.72	B	C
ATOM	3889	CB	TYR	B	265	18.812	97.062	27.862	1.00	30.64	B	C
ATOM	3890	CG	TYR	B	265	18.411	97.430	29.280	1.00	29.22	B	C
ATOM	3891	CD1	TYR	B	265	19.212	97.123	30.383	1.00	29.05	B	C
ATOM	3892	CE1	TYR	B	265	18.847	97.542	31.669	1.00	29.36	B	C
ATOM	3893	CD2	TYR	B	265	17.247	98.148	29.507	1.00	28.66	B	C
ATOM	3894	CE2	TYR	B	265	16.881	98.564	30.773	1.00	28.08	B	C
ATOM	3895	CZ	TYR	B	265	17.670	98.272	31.844	1.00	28.00	B	C
ATOM	3896	OH	TYR	B	265	17.249	98.790	33.044	1.00	26.33	B	O
ATOM	3897	C	TYR	B	265	17.078	95.212	27.538	1.00	14.87	B	C
ATOM	3898	O	TYR	B	265	16.166	95.816	26.981	1.00	15.19	B	O
ATOM	3899	N	PRO	B	266	16.861	94.146	28.321	1.00	46.31	B	N
ATOM	3900	CD	PRO	B	266	18.010	93.599	29.051	1.00	59.76	B	C
ATOM	3901	CA	PRO	B	266	15.645	93.439	28.732	1.00	48.14	B	C
ATOM	3902	CB	PRO	B	266	16.147	92.484	29.817	1.00	62.25	B	C
ATOM	3903	CG	PRO	B	266	17.363	93.155	30.326	1.00	60.79	B	C
ATOM	3904	C	PRO	B	266	14.412	94.207	29.181	1.00	53.79	B	C
ATOM	3905	O	PRO	B	266	13.468	94.332	28.417	1.00	55.38	B	O
ATOM	3906	N	ILE	B	267	14.399	94.695	30.415	1.00	84.19	B	N
ATOM	3907	CA	ILE	B	267	13.230	95.409	30.927	1.00	85.33	B	C

ATOM	3908	CB	ILE	B	267	13.628	96.575	31.852	1.00 64.71	B	C
ATOM	3909	CG2	ILE	B	267	12.404	97.437	32.130	1.00 63.60	B	C
ATOM	3910	CG1	ILE	B	267	14.244	96.048	33.151	1.00 63.57	B	C
ATOM	3911	CD1	ILE	B	267	15.690	95.698	33.037	1.00 62.63	B	C
ATOM	3912	C	ILE	B	267	12.277	95.963	29.855	1.00 90.38	B	C
ATOM	3913	O	ILE	B	267	11.138	95.501	29.717	1.00 90.46	B	O
ATOM	3914	N	PRO	B	268	12.728	96.965	29.085	1.00 53.14	B	N
ATOM	3915	CD	PRO	B	268	14.052	97.609	29.123	1.00 37.36	B	C
ATOM	3916	CA	PRO	B	268	11.883	97.556	28.035	1.00 52.48	B	C
ATOM	3917	CB	PRO	B	268	12.786	98.633	27.439	1.00 40.91	B	C
ATOM	3918	CG	PRO	B	268	13.737	98.965	28.576	1.00 38.83	B	C
ATOM	3919	C	PRO	B	268	11.495	96.488	27.011	1.00 57.30	B	C
ATOM	3920	O	PRO	B	268	12.146	95.452	26.927	1.00 57.14	B	O
ATOM	3921	N	PRO	B	269	10.476	96.755	26.178	1.00174.81	B	N
ATOM	3922	CD	PRO	B	269	10.221	98.118	25.674	1.00105.34	B	C
ATOM	3923	CA	PRO	B	269	10.044	95.770	25.182	1.00173.67	B	C
ATOM	3924	CB	PRO	B	269	10.266	96.513	23.877	1.00107.01	B	C
ATOM	3925	CG	PRO	B	269	9.739	97.875	24.230	1.00106.77	B	C
ATOM	3926	C	PRO	B	269	10.775	94.429	25.245	1.00176.77	B	C
ATOM	3927	O	PRO	B	269	11.619	94.131	24.399	1.00177.52	B	O
ATOM	3928	N	PRO	B	270	10.466	93.607	26.267	1.00 67.66	B	N
ATOM	3929	CD	PRO	B	270	9.648	93.877	27.467	1.00 53.56	B	C
ATOM	3930	CA	PRO	B	270	11.124	92.310	26.391	1.00 65.29	B	C
ATOM	3931	CB	PRO	B	270	10.509	91.743	27.676	1.00 54.95	B	C
ATOM	3932	CG	PRO	B	270	10.276	92.968	28.507	1.00 54.76	B	C
ATOM	3933	C	PRO	B	270	10.904	91.405	25.183	1.00 65.93	B	C
ATOM	3934	O	PRO	B	270	11.716	91.375	24.255	1.00 64.07	B	O
ATOM	3935	N	ASP	B	271	9.785	90.688	25.208	1.00 66.78	B	N
ATOM	3936	CA	ASP	B	271	9.421	89.740	24.160	1.00 65.63	B	C
ATOM	3937	CB	ASP	B	271	8.358	88.791	24.701	1.00120.82	B	C
ATOM	3938	CG	ASP	B	271	8.718	88.246	26.069	1.00121.57	B	C
ATOM	3939	OD1	ASP	B	271	7.874	87.548	26.674	1.00121.31	B	O
ATOM	3940	OD2	ASP	B	271	9.847	88.518	26.537	1.00122.22	B	O
ATOM	3941	C	ASP	B	271	8.930	90.375	22.864	1.00 66.41	B	C
ATOM	3942	O	ASP	B	271	9.365	91.468	22.485	1.00 65.99	B	O
ATOM	3943	N	ALA	B	272	8.032	89.669	22.183	1.00100.50	B	N
ATOM	3944	CA	ALA	B	272	7.465	90.144	20.924	1.00100.34	B	C
ATOM	3945	CB	ALA	B	272	6.669	91.430	21.159	1.00148.84	B	C
ATOM	3946	C	ALA	B	272	8.556	90.378	19.879	1.00101.41	B	C
ATOM	3947	O	ALA	B	272	9.101	91.482	19.760	1.00101.59	B	O
ATOM	3948	N	LYS	B	273	8.862	89.328	19.121	1.00 80.04	B	N
ATOM	3949	CA	LYS	B	273	9.893	89.393	18.094	1.00 81.18	B	C
ATOM	3950	CB	LYS	B	273	9.985	88.059	17.346	1.00 72.72	B	C

ATOM	3951	CG	LYS	B	273	9.996	86.818	18.230	1.00 72.43	B	C
ATOM	3952	CD	LYS	B	273	10.043	85.565	17.369	1.00 73.66	B	C
ATOM	3953	CE	LYS	B	273	9.552	84.314	18.109	1.00 75.67	B	C
ATOM	3954	NZ	LYS	B	273	10.457	83.820	19.191	1.00 76.42	B	N
ATOM	3955	C	LYS	B	273	9.597	90.509	17.103	1.00 81.16	B	C
ATOM	3956	O	LYS	B	273	10.470	90.912	16.335	1.00 80.63	B	O
ATOM	3957	N	ASP	B	311	10.335	99.628	18.017	1.00106.32	B	N
ATOM	3958	CA	ASP	B	311	10.523	98.186	17.913	1.00107.34	B	C
ATOM	3959	CB	ASP	B	311	9.816	97.653	16.656	1.00186.18	B	C
ATOM	3960	CG	ASP	B	311	10.392	98.223	15.365	1.00185.92	B	C
ATOM	3961	OD1	ASP	B	311	9.783	98.006	14.293	1.00185.00	B	O
ATOM	3962	OD2	ASP	B	311	11.453	98.879	15.415	1.00185.85	B	O
ATOM	3963	C	ASP	B	311	12.008	97.824	17.877	1.00107.36	B	C
ATOM	3964	O	ASP	B	311	12.673	97.766	18.914	1.00107.37	B	O
ATOM	3965	N	SER	B	312	12.426	101.290	15.047	1.00197.00	B	N
ATOM	3966	CA	SER	B	312	12.174	101.436	16.475	1.00195.63	B	C
ATOM	3967	CB	SER	B	312	13.495	101.646	17.224	1.00117.65	B	C
ATOM	3968	OG	SER	B	312	14.372	100.547	17.044	1.00117.53	B	O
ATOM	3969	C	SER	B	312	11.233	102.606	16.758	1.00194.49	B	C
ATOM	3970	O	SER	B	312	11.023	103.469	15.905	1.00193.66	B	O
ATOM	3971	N	ARG	B	313	10.662	102.622	17.958	1.00203.67	B	N
ATOM	3972	CA	ARG	B	313	9.758	103.691	18.362	1.00202.73	B	C
ATOM	3973	CB	ARG	B	313	8.295	103.261	18.178	1.00154.97	B	C
ATOM	3974	CG	ARG	B	313	7.856	102.024	18.961	1.00155.74	B	C
ATOM	3975	CD	ARG	B	313	7.036	102.396	20.193	1.00156.10	B	C
ATOM	3976	NE	ARG	B	313	7.872	102.652	21.361	1.00157.28	B	N
ATOM	3977	CZ	ARG	B	313	8.479	101.701	22.062	1.00157.78	B	C
ATOM	3978	NH1	ARG	B	313	8.338	100.429	21.717	1.00157.11	B	N
ATOM	3979	NH2	ARG	B	313	9.238	102.017	23.101	1.00157.69	B	N
ATOM	3980	C	ARG	B	313	10.030	104.082	19.810	1.00199.44	B	C
ATOM	3981	O	ARG	B	313	10.466	103.262	20.617	1.00198.75	B	O
ATOM	3982	N	PRO	B	314	9.795	105.357	20.147	1.00193.99	B	N
ATOM	3983	CD	PRO	B	314	9.554	106.423	19.161	1.00149.20	B	C
ATOM	3984	CA	PRO	B	314	10.000	105.925	21.486	1.00190.52	B	C
ATOM	3985	CB	PRO	B	314	9.887	107.432	21.244	1.00147.46	B	C
ATOM	3986	CG	PRO	B	314	10.263	107.585	19.792	1.00148.35	B	C
ATOM	3987	C	PRO	B	314	9.028	105.455	22.573	1.00186.55	B	C
ATOM	3988	O	PRO	B	314	7.892	105.072	22.286	1.00185.60	B	O
ATOM	3989	N	ALA	B	315	9.495	105.504	23.819	1.00 96.94	B	N
ATOM	3990	CA	ALA	B	315	8.703	105.121	24.990	1.00 92.71	B	C
ATOM	3991	CB	ALA	B	315	7.886	103.855	24.709	1.00 98.38	B	C
ATOM	3992	C	ALA	B	315	9.611	104.900	26.194	1.00 89.91	B	C
ATOM	3993	O	ALA	B	315	10.779	105.305	26.183	1.00 90.08	B	O

ATOM	3994	N	MET	B	316	9.066	104.244	27.217	1.00 88.35	B	N
ATOM	3995	CA	MET	B	316	9.796	103.972	28.448	1.00 83.95	B	C
ATOM	3996	CB	MET	B	316	10.599	102.678	28.327	1.00106.05	B	C
ATOM	3997	CG	MET	B	316	9.829	101.452	28.788	1.00100.73	B	C
ATOM	3998	SD	MET	B	316	9.662	101.358	30.595	1.00 97.17	B	S
ATOM	3999	CE	MET	B	316	9.558	99.537	30.844	1.00 98.91	B	C
ATOM	4000	C	MET	B	316	10.711	105.128	28.794	1.00 82.47	B	C
ATOM	4001	O	MET	B	316	11.855	105.198	28.337	1.00 82.89	B	O
ATOM	4002	N	ALA	B	317	10.185	106.049	29.592	1.00 75.04	B	N
ATOM	4003	CA	ALA	B	317	10.948	107.206	30.006	1.00 72.83	B	C
ATOM	4004	CB	ALA	B	317	10.033	108.275	30.541	1.00 59.22	B	C
ATOM	4005	C	ALA	B	317	11.924	106.774	31.076	1.00 70.40	B	C
ATOM	4006	O	ALA	B	317	12.931	106.142	30.773	1.00 70.17	B	O
ATOM	4007	N	ILE	B	318	11.634	107.123	32.327	1.00 54.47	B	N
ATOM	4008	CA	ILE	B	318	12.518	106.786	33.441	1.00 55.06	B	C
ATOM	4009	CB	ILE	B	318	13.374	107.982	33.871	1.00 54.35	B	C
ATOM	4010	CG2	ILE	B	318	14.095	107.666	35.172	1.00 54.41	B	C
ATOM	4011	CG1	ILE	B	318	14.344	108.338	32.752	1.00 55.21	B	C
ATOM	4012	CD1	ILE	B	318	13.637	108.741	31.467	1.00 57.32	B	C
ATOM	4013	C	ILE	B	318	11.760	106.331	34.663	1.00 54.22	B	C
ATOM	4014	O	ILE	B	318	12.074	105.305	35.257	1.00 54.02	B	O
ATOM	4015	N	PHE	B	319	10.778	107.119	35.065	1.00 68.33	B	N
ATOM	4016	CA	PHE	B	319	9.991	106.752	36.220	1.00 66.89	B	C
ATOM	4017	CB	PHE	B	319	8.880	107.769	36.470	1.00 48.73	B	C
ATOM	4018	CG	PHE	B	319	8.105	107.522	37.729	1.00 46.03	B	C
ATOM	4019	CD1	PHE	B	319	6.731	107.634	37.743	1.00 45.39	B	C
ATOM	4020	CD2	PHE	B	319	8.759	107.208	38.907	1.00 46.37	B	C
ATOM	4021	CE1	PHE	B	319	6.023	107.439	38.913	1.00 45.40	B	C
ATOM	4022	CE2	PHE	B	319	8.054	107.013	40.081	1.00 45.72	B	C
ATOM	4023	CZ	PHE	B	319	6.685	107.128	40.084	1.00 44.55	B	C
ATOM	4024	C	PHE	B	319	9.369	105.422	35.871	1.00 65.65	B	C
ATOM	4025	O	PHE	B	319	9.395	104.497	36.678	1.00 64.02	B	O
ATOM	4026	N	GLU	B	320	8.822	105.343	34.655	1.00 52.00	B	N
ATOM	4027	CA	GLU	B	320	8.162	104.135	34.151	1.00 53.56	B	C
ATOM	4028	CB	GLU	B	320	7.652	104.361	32.720	1.00104.89	B	C
ATOM	4029	CG	GLU	B	320	6.465	103.480	32.334	1.00109.29	B	C
ATOM	4030	CD	GLU	B	320	6.592	102.883	30.945	1.00111.61	B	C
ATOM	4031	OE1	GLU	B	320	6.955	103.623	30.007	1.00113.18	B	O
ATOM	4032	OE2	GLU	B	320	6.319	101.674	30.794	1.00111.83	B	O
ATOM	4033	C	GLU	B	320	9.160	102.989	34.161	1.00 52.52	B	C
ATOM	4034	O	GLU	B	320	8.902	101.920	34.719	1.00 53.17	B	O
ATOM	4035	N	LEU	B	321	10.303	103.224	33.526	1.00 50.82	B	N
ATOM	4036	CA	LEU	B	321	11.356	102.232	33.489	1.00 49.87	B	C

ATOM	4037	CB	LEU	B	321	12.575	102.807	32.794	1.00	31.85	B	C
ATOM	4038	CG	LEU	B	321	13.886	102.320	33.385	1.00	32.12	B	C
ATOM	4039	CD1	LEU	B	321	14.916	102.135	32.282	1.00	32.19	B	C
ATOM	4040	CD2	LEU	B	321	14.352	103.315	34.424	1.00	31.49	B	C
ATOM	4041	C	LEU	B	321	11.696	101.827	34.919	1.00	47.94	B	C
ATOM	4042	O	LEU	B	321	11.879	100.649	35.212	1.00	44.93	B	O
ATOM	4043	N	LEU	B	322	11.771	102.811	35.808	1.00	34.81	B	N
ATOM	4044	CA	LEU	B	322	12.055	102.565	37.218	1.00	35.00	B	C
ATOM	4045	CB	LEU	B	322	12.367	103.888	37.920	1.00	24.26	B	C
ATOM	4046	CG	LEU	B	322	13.756	104.095	38.543	1.00	25.22	B	C
ATOM	4047	CD1	LEU	B	322	14.874	104.057	37.499	1.00	27.70	B	C
ATOM	4048	CD2	LEU	B	322	13.749	105.447	39.239	1.00	28.16	B	C
ATOM	4049	C	LEU	B	322	10.850	101.885	37.889	1.00	35.99	B	C
ATOM	4050	O	LEU	B	322	11.007	101.056	38.785	1.00	33.40	B	O
ATOM	4051	N	ASP	B	323	9.644	102.239	37.453	1.00	75.87	B	N
ATOM	4052	CA	ASP	B	323	8.427	101.645	38.005	1.00	76.74	B	C
ATOM	4053	CB	ASP	B	323	7.176	102.395	37.524	1.00	80.08	B	C
ATOM	4054	CG	ASP	B	323	5.874	101.705	37.941	1.00	82.78	B	C
ATOM	4055	OD1	ASP	B	323	5.516	101.757	39.136	1.00	84.64	B	O
ATOM	4056	OD2	ASP	B	323	5.210	101.105	37.069	1.00	82.19	B	O
ATOM	4057	C	ASP	B	323	8.351	100.210	37.529	1.00	77.01	B	C
ATOM	4058	O	ASP	B	323	8.035	99.303	38.297	1.00	77.75	B	O
ATOM	4059	N	TYR	B	324	8.639	100.008	36.249	1.00	69.52	B	N
ATOM	4060	CA	TYR	B	324	8.595	98.671	35.702	1.00	69.52	B	C
ATOM	4061	CB	TYR	B	324	9.154	98.633	34.282	1.00	74.68	B	C
ATOM	4062	CG	TYR	B	324	8.896	97.308	33.600	1.00	76.69	B	C
ATOM	4063	CD1	TYR	B	324	7.898	97.176	32.645	1.00	76.94	B	C
ATOM	4064	CE1	TYR	B	324	7.622	95.957	32.071	1.00	76.54	B	C
ATOM	4065	CD2	TYR	B	324	9.612	96.176	33.958	1.00	77.28	B	C
ATOM	4066	CE2	TYR	B	324	9.341	94.954	33.393	1.00	77.93	B	C
ATOM	4067	CZ	TYR	B	324	8.345	94.847	32.451	1.00	77.26	B	C
ATOM	4068	OH	TYR	B	324	8.070	93.615	31.899	1.00	78.90	B	O
ATOM	4069	C	TYR	B	324	9.470	97.838	36.605	1.00	69.42	B	C
ATOM	4070	O	TYR	B	324	8.991	96.977	37.339	1.00	68.09	B	O
ATOM	4071	N	ILE	B	325	10.761	98.136	36.553	1.00	41.08	B	N
ATOM	4072	CA	ILE	B	325	11.768	97.449	37.340	1.00	37.89	B	C
ATOM	4073	CB	ILE	B	325	13.047	98.284	37.391	1.00	15.26	B	C
ATOM	4074	CG2	ILE	B	325	13.963	97.786	38.477	1.00	17.35	B	C
ATOM	4075	CG1	ILE	B	325	13.729	98.251	36.034	1.00	14.03	B	C
ATOM	4076	CD1	ILE	B	325	14.811	99.290	35.902	1.00	13.82	B	C
ATOM	4077	C	ILE	B	325	11.382	97.078	38.769	1.00	39.20	B	C
ATOM	4078	O	ILE	B	325	11.278	95.893	39.088	1.00	39.63	B	O
ATOM	4079	N	VAL	B	326	11.153	98.078	39.622	1.00	57.64	B	N

ATOM	4080	CA	VAL	B	326	10.846	97.810	41.031	1.00	57.87	B C
ATOM	4081	CB	VAL	B	326	10.843	99.099	41.910	1.00	39.98	B C
ATOM	4082	CG1	VAL	B	326	11.859	100.111	41.395	1.00	38.18	B C
ATOM	4083	CG2	VAL	B	326	9.455	99.668	41.976	1.00	40.71	B C
ATOM	4084	C	VAL	B	326	9.557	97.075	41.338	1.00	60.66	B C
ATOM	4085	O	VAL	B	326	9.293	96.778	42.503	1.00	61.79	B O
ATOM	4086	N	ASN	B	327	8.750	96.767	40.329	1.00	52.16	B N
ATOM	4087	CA	ASN	B	327	7.514	96.068	40.641	1.00	52.86	B C
ATOM	4088	CB	ASN	B	327	6.649	96.937	41.553	1.00	53.39	B C
ATOM	4089	CG	ASN	B	327	6.403	98.298	40.973	1.00	57.15	B C
ATOM	4090	OD1	ASN	B	327	6.163	98.434	39.773	1.00	57.98	B O
ATOM	4091	ND2	ASN	B	327	6.455	99.320	41.818	1.00	56.60	B N
ATOM	4092	C	ASN	B	327	6.611	95.522	39.550	1.00	52.13	B C
ATOM	4093	O	ASN	B	327	5.400	95.619	39.701	1.00	52.24	B O
ATOM	4094	N	GLU	B	328	7.162	94.956	38.476	1.00	62.44	B N
ATOM	4095	CA	GLU	B	328	6.303	94.365	37.451	1.00	61.82	B C
ATOM	4096	CB	GLU	B	328	5.025	95.174	37.279	1.00	189.08	B C
ATOM	4097	CG	GLU	B	328	3.965	94.448	36.480	1.00	189.15	B C
ATOM	4098	CD	GLU	B	328	3.102	95.391	35.679	1.00	189.52	B C
ATOM	4099	OE1	GLU	B	328	2.632	96.396	36.250	1.00	188.49	B O
ATOM	4100	OE2	GLU	B	328	2.892	95.125	34.477	1.00	192.55	B O
ATOM	4101	C	GLU	B	328	6.848	94.118	36.052	1.00	61.66	B C
ATOM	4102	O	GLU	B	328	6.553	94.903	35.150	1.00	61.80	B O
ATOM	4103	N	PRO	B	329	7.655	93.067	35.854	1.00	64.88	B N
ATOM	4104	CD	PRO	B	329	7.161	92.472	34.587	1.00	27.73	B C
ATOM	4105	CA	PRO	B	329	8.256	91.984	36.629	1.00	67.10	B C
ATOM	4106	CB	PRO	B	329	7.270	90.854	36.423	1.00	28.60	B C
ATOM	4107	CG	PRO	B	329	6.985	90.961	34.946	1.00	28.32	B C
ATOM	4108	C	PRO	B	329	9.611	91.733	35.934	1.00	67.64	B C
ATOM	4109	O	PRO	B	329	9.921	92.379	34.928	1.00	66.60	B O
ATOM	4110	N	PRO	B	330	10.416	90.780	36.430	1.00	35.83	B N
ATOM	4111	CD	PRO	B	330	10.085	89.806	37.481	1.00	54.51	B C
ATOM	4112	CA	PRO	B	330	11.727	90.478	35.838	1.00	38.95	B C
ATOM	4113	CB	PRO	B	330	12.263	89.383	36.751	1.00	55.11	B C
ATOM	4114	CG	PRO	B	330	11.022	88.674	37.163	1.00	53.74	B C
ATOM	4115	C	PRO	B	330	11.732	90.079	34.364	1.00	40.48	B C
ATOM	4116	O	PRO	B	330	10.781	89.477	33.873	1.00	40.85	B O
ATOM	4117	N	PRO	B	331	12.816	90.423	33.642	1.00	57.05	B N
ATOM	4118	CD	PRO	B	331	13.895	91.251	34.205	1.00	80.91	B C
ATOM	4119	CA	PRO	B	331	13.070	90.168	32.220	1.00	58.95	B C
ATOM	4120	CB	PRO	B	331	14.513	90.604	32.054	1.00	81.97	B C
ATOM	4121	CG	PRO	B	331	14.568	91.784	32.955	1.00	81.78	B C
ATOM	4122	C	PRO	B	331	12.845	88.733	31.807	1.00	61.16	B C

ATOM	4123	O	PRO	B	331	11.698	88.341	31.599	1.00	61.70	B	O
ATOM	4124	N	LYS	B	332	13.930	87.968	31.666	1.00	66.13	B	N
ATOM	4125	CA	LYS	B	332	13.865	86.550	31.292	1.00	66.58	B	C
ATOM	4126	CB	LYS	B	332	12.464	86.007	31.547	1.00	40.79	B	C
ATOM	4127	CG	LYS	B	332	12.202	84.638	31.021	1.00	42.68	B	C
ATOM	4128	CD	LYS	B	332	10.842	84.202	31.507	1.00	44.54	B	C
ATOM	4129	CE	LYS	B	332	9.779	85.261	31.183	1.00	43.24	B	C
ATOM	4130	NZ	LYS	B	332	9.549	85.460	29.715	1.00	43.39	B	N
ATOM	4131	C	LYS	B	332	14.291	86.190	29.871	1.00	67.01	B	C
ATOM	4132	O	LYS	B	332	14.017	86.918	28.924	1.00	67.78	B	O
ATOM	4133	N	LEU	B	333	14.957	85.044	29.744	1.00	45.26	B	N
ATOM	4134	CA	LEU	B	333	15.451	84.542	28.468	1.00	46.81	B	C
ATOM	4135	CB	LEU	B	333	16.657	83.631	28.678	1.00	39.71	B	C
ATOM	4136	CG	LEU	B	333	17.995	84.195	29.136	1.00	38.43	B	C
ATOM	4137	CD1	LEU	B	333	18.974	83.055	29.359	1.00	37.75	B	C
ATOM	4138	CD2	LEU	B	333	18.528	85.148	28.087	1.00	37.96	B	C
ATOM	4139	C	LEU	B	333	14.392	83.738	27.756	1.00	48.33	B	C
ATOM	4140	O	LEU	B	333	13.713	82.915	28.372	1.00	46.97	B	O
ATOM	4141	N	PRO	B	334	14.250	83.953	26.437	1.00	55.01	B	N
ATOM	4142	CD	PRO	B	334	15.058	84.886	25.632	1.00	69.65	B	C
ATOM	4143	CA	PRO	B	334	13.272	83.246	25.601	1.00	56.11	B	C
ATOM	4144	CB	PRO	B	334	13.457	83.895	24.230	1.00	69.44	B	C
ATOM	4145	CG	PRO	B	334	14.900	84.324	24.245	1.00	69.83	B	C
ATOM	4146	C	PRO	B	334	13.587	81.753	25.598	1.00	57.43	B	C
ATOM	4147	O	PRO	B	334	14.590	81.315	25.033	1.00	59.43	B	O
ATOM	4148	N	ASN	B	335	12.731	80.975	26.248	1.00	63.56	B	N
ATOM	4149	CA	ASN	B	335	12.948	79.539	26.344	1.00	63.37	B	C
ATOM	4150	CB	ASN	B	335	11.888	78.897	27.239	1.00	74.06	B	C
ATOM	4151	CG	ASN	B	335	10.505	79.002	26.667	1.00	75.49	B	C
ATOM	4152	OD1	ASN	B	335	9.568	78.381	27.165	1.00	76.90	B	O
ATOM	4153	ND2	ASN	B	335	10.362	79.795	25.615	1.00	74.62	B	N
ATOM	4154	C	ASN	B	335	12.937	78.856	24.992	1.00	62.53	B	C
ATOM	4155	O	ASN	B	335	12.075	78.021	24.725	1.00	62.14	B	O
ATOM	4156	N	GLY	B	336	13.904	79.187	24.146	1.00	51.39	B	N
ATOM	4157	CA	GLY	B	336	13.930	78.581	22.830	1.00	49.29	B	C
ATOM	4158	C	GLY	B	336	15.272	78.060	22.372	1.00	47.99	B	C
ATOM	4159	O	GLY	B	336	15.448	76.854	22.192	1.00	49.17	B	O
ATOM	4160	N	VAL	B	337	16.217	78.972	22.173	1.00	118.38	B	N
ATOM	4161	CA	VAL	B	337	17.545	78.592	21.721	1.00	117.55	B	C
ATOM	4162	CB	VAL	B	337	18.121	79.651	20.782	1.00	84.33	B	C
ATOM	4163	CG1	VAL	B	337	18.228	80.978	21.507	1.00	84.95	B	C
ATOM	4164	CG2	VAL	B	337	19.475	79.199	20.271	1.00	84.78	B	C
ATOM	4165	C	VAL	B	337	18.526	78.364	22.872	1.00	117.03	B	C

ATOM	4166	O	VAL	B	337	19.490	77.609	22.726	1.00118.63	B	O
ATOM	4167	N	PHE	B	338	18.287	79.009	24.011	1.00 53.61	B	N
ATOM	4168	CA	PHE	B	338	19.163	78.835	25.162	1.00 52.21	B	C
ATOM	4169	CB	PHE	B	338	19.089	80.039	26.083	1.00 53.41	B	C
ATOM	4170	CG	PHE	B	338	19.447	81.323	25.418	1.00 50.16	B	C
ATOM	4171	CD1	PHE	B	338	18.531	81.986	24.629	1.00 50.41	B	C
ATOM	4172	CD2	PHE	B	338	20.707	81.873	25.583	1.00 48.27	B	C
ATOM	4173	CE1	PHE	B	338	18.864	83.178	24.016	1.00 51.22	B	C
ATOM	4174	CE2	PHE	B	338	21.045	83.066	24.971	1.00 47.35	B	C
ATOM	4175	CZ	PHE	B	338	20.122	83.720	24.187	1.00 49.01	B	C
ATOM	4176	C	PHE	B	338	18.759	77.598	25.934	1.00 52.89	B	C
ATOM	4177	O	PHE	B	338	17.570	77.367	26.160	1.00 54.40	B	O
ATOM	4178	N	THR	B	339	19.756	76.813	26.343	1.00 47.54	B	N
ATOM	4179	CA	THR	B	339	19.530	75.575	27.089	1.00 49.17	B	C
ATOM	4180	CB	THR	B	339	20.840	74.878	27.446	1.00 49.64	B	C
ATOM	4181	OG1	THR	B	339	21.435	75.535	28.571	1.00 52.26	B	O
ATOM	4182	CG2	THR	B	339	21.799	74.918	26.263	1.00 47.04	B	C
ATOM	4183	C	THR	B	339	18.789	75.831	28.382	1.00 49.40	B	C
ATOM	4184	O	THR	B	339	18.994	76.846	29.048	1.00 49.28	B	O
ATOM	4185	N	PRO	B	340	17.935	74.888	28.766	1.00 45.72	B	N
ATOM	4186	CD	PRO	B	340	17.927	73.539	28.191	1.00 39.93	B	C
ATOM	4187	CA	PRO	B	340	17.117	74.942	29.976	1.00 46.42	B	C
ATOM	4188	CB	PRO	B	340	16.714	73.492	30.186	1.00 42.21	B	C
ATOM	4189	CG	PRO	B	340	16.680	72.962	28.799	1.00 41.97	B	C
ATOM	4190	C	PRO	B	340	17.892	75.487	31.159	1.00 46.60	B	C
ATOM	4191	O	PRO	B	340	17.544	76.529	31.713	1.00 48.23	B	O
ATOM	4192	N	ASP	B	341	18.955	74.784	31.538	1.00 63.66	B	N
ATOM	4193	CA	ASP	B	341	19.771	75.194	32.674	1.00 65.05	B	C
ATOM	4194	CB	ASP	B	341	20.940	74.230	32.833	1.00 57.12	B	C
ATOM	4195	CG	ASP	B	341	20.482	72.833	33.163	1.00 57.70	B	C
ATOM	4196	OD1	ASP	B	341	19.754	72.664	34.160	1.00 59.21	B	O
ATOM	4197	OD2	ASP	B	341	20.845	71.901	32.426	1.00 56.17	B	O
ATOM	4198	C	ASP	B	341	20.272	76.638	32.623	1.00 65.13	B	C
ATOM	4199	O	ASP	B	341	20.401	77.285	33.664	1.00 66.29	B	O
ATOM	4200	N	PHE	B	342	20.559	77.146	31.425	1.00 34.05	B	N
ATOM	4201	CA	PHE	B	342	21.022	78.518	31.311	1.00 33.02	B	C
ATOM	4202	CB	PHE	B	342	21.534	78.836	29.922	1.00 30.86	B	C
ATOM	4203	CG	PHE	B	342	21.992	80.252	29.779	1.00 30.79	B	C
ATOM	4204	CD1	PHE	B	342	22.379	80.975	30.888	1.00 31.45	B	C
ATOM	4205	CD2	PHE	B	342	22.084	80.847	28.543	1.00 31.23	B	C
ATOM	4206	CE1	PHE	B	342	22.848	82.251	30.766	1.00 32.91	B	C
ATOM	4207	CE2	PHE	B	342	22.558	82.134	28.418	1.00 30.82	B	C
ATOM	4208	CZ	PHE	B	342	22.940	82.832	29.531	1.00 32.45	B	C

ATOM	4209	C	PHE	B	342	19.842	79.387	31.591	1.00	31.67	B	C
ATOM	4210	O	PHE	B	342	19.974	80.465	32.155	1.00	31.63	B	O
ATOM	4211	N	GLN	B	343	18.683	78.908	31.165	1.00	14.25	B	N
ATOM	4212	CA	GLN	B	343	17.437	79.607	31.391	1.00	14.50	B	C
ATOM	4213	CB	GLN	B	343	16.320	78.800	30.754	1.00	93.57	B	C
ATOM	4214	CG	GLN	B	343	14.968	79.445	30.704	1.00	93.76	B	C
ATOM	4215	CD	GLN	B	343	13.958	78.493	30.113	1.00	94.46	B	C
ATOM	4216	OE1	GLN	B	343	13.174	77.867	30.829	1.00	94.65	B	O
ATOM	4217	NE2	GLN	B	343	13.996	78.347	28.797	1.00	95.10	B	N
ATOM	4218	C	GLN	B	343	17.243	79.702	32.919	1.00	13.98	B	C
ATOM	4219	O	GLN	B	343	17.126	80.780	33.492	1.00	15.07	B	O
ATOM	4220	N	GLU	B	344	17.248	78.552	33.572	1.00	31.95	B	N
ATOM	4221	CA	GLU	B	344	17.077	78.451	35.017	1.00	32.03	B	C
ATOM	4222	CB	GLU	B	344	17.196	76.979	35.390	1.00	60.95	B	C
ATOM	4223	CG	GLU	B	344	16.956	76.640	36.827	1.00	67.95	B	C
ATOM	4224	CD	GLU	B	344	16.706	75.157	36.991	1.00	71.66	B	C
ATOM	4225	OE1	GLU	B	344	16.602	74.690	38.145	1.00	73.03	B	O
ATOM	4226	OE2	GLU	B	344	16.605	74.460	35.955	1.00	72.33	B	O
ATOM	4227	C	GLU	B	344	18.043	79.289	35.869	1.00	29.44	B	C
ATOM	4228	O	GLU	B	344	17.685	79.729	36.954	1.00	30.33	B	O
ATOM	4229	N	PHE	B	345	19.259	79.498	35.371	1.00	37.02	B	N
ATOM	4230	CA	PHE	B	345	20.300	80.254	36.067	1.00	34.44	B	C
ATOM	4231	CB	PHE	B	345	21.641	79.915	35.426	1.00	8.25	B	C
ATOM	4232	CG	PHE	B	345	22.787	80.779	35.876	1.00	6.37	B	C
ATOM	4233	CD1	PHE	B	345	23.546	80.436	36.979	1.00	5.49	B	C
ATOM	4234	CD2	PHE	B	345	23.141	81.903	35.153	1.00	6.58	B	C
ATOM	4235	CE1	PHE	B	345	24.638	81.201	37.340	1.00	4.67	B	C
ATOM	4236	CE2	PHE	B	345	24.221	82.657	35.511	1.00	7.90	B	C
ATOM	4237	CZ	PHE	B	345	24.977	82.308	36.607	1.00	5.88	B	C
ATOM	4238	C	PHE	B	345	20.090	81.774	36.087	1.00	34.75	B	C
ATOM	4239	O	PHE	B	345	20.408	82.431	37.083	1.00	34.02	B	O
ATOM	4240	N	VAL	B	346	19.576	82.342	34.997	1.00	31.29	B	N
ATOM	4241	CA	VAL	B	346	19.334	83.781	34.973	1.00	31.56	B	C
ATOM	4242	CB	VAL	B	346	19.316	84.371	33.546	1.00	16.03	B	C
ATOM	4243	CG1	VAL	B	346	20.621	84.053	32.836	1.00	17.70	B	C
ATOM	4244	CG2	VAL	B	346	18.109	83.859	32.777	1.00	17.48	B	C
ATOM	4245	C	VAL	B	346	17.998	84.071	35.634	1.00	31.79	B	C
ATOM	4246	O	VAL	B	346	17.783	85.159	36.152	1.00	32.96	B	O
ATOM	4247	N	ASN	B	347	17.092	83.101	35.614	1.00	26.87	B	N
ATOM	4248	CA	ASN	B	347	15.814	83.306	36.255	1.00	28.12	B	C
ATOM	4249	CB	ASN	B	347	14.866	82.146	35.983	1.00	59.52	B	C
ATOM	4250	CG	ASN	B	347	14.050	82.347	34.734	1.00	59.58	B	C
ATOM	4251	OD1	ASN	B	347	14.593	82.575	33.661	1.00	56.61	B	O

ATOM	4252	ND2	ASN	B	347	12.736	82.261	34.864	1.00	61.19	B	N
ATOM	4253	C	ASN	B	347	16.151	83.360	37.724	1.00	28.81	B	C
ATOM	4254	O	ASN	B	347	15.412	83.947	38.520	1.00	30.06	B	O
ATOM	4255	N	LYS	B	348	17.285	82.752	38.074	1.00	27.37	B	N
ATOM	4256	CA	LYS	B	348	17.746	82.695	39.458	1.00	30.26	B	C
ATOM	4257	CB	LYS	B	348	18.891	81.700	39.596	1.00	51.60	B	C
ATOM	4258	CG	LYS	B	348	18.490	80.252	39.465	1.00	54.51	B	C
ATOM	4259	CD	LYS	B	348	17.429	79.877	40.473	1.00	57.23	B	C
ATOM	4260	CE	LYS	B	348	17.335	78.368	40.610	1.00	60.31	B	C
ATOM	4261	NZ	LYS	B	348	18.620	77.787	41.106	1.00	60.32	B	N
ATOM	4262	C	LYS	B	348	18.209	84.038	39.972	1.00	30.37	B	C
ATOM	4263	O	LYS	B	348	17.891	84.425	41.099	1.00	30.86	B	O
ATOM	4264	N	CYS	B	349	18.963	84.734	39.127	1.00	47.77	B	N
ATOM	4265	CA	CYS	B	349	19.518	86.045	39.445	1.00	45.76	B	C
ATOM	4266	CB	CYS	B	349	20.691	86.342	38.522	1.00	43.22	B	C
ATOM	4267	SG	CYS	B	349	21.692	84.916	38.231	1.00	43.51	B	S
ATOM	4268	C	CYS	B	349	18.510	87.175	39.317	1.00	46.22	B	C
ATOM	4269	O	CYS	B	349	18.614	88.179	40.012	1.00	47.91	B	O
ATOM	4270	N	LEU	B	350	17.545	87.009	38.421	1.00	42.73	B	N
ATOM	4271	CA	LEU	B	350	16.536	88.028	38.186	1.00	43.37	B	C
ATOM	4272	CB	LEU	B	350	16.008	87.918	36.756	1.00	25.64	B	C
ATOM	4273	CG	LEU	B	350	16.442	88.905	35.667	1.00	25.64	B	C
ATOM	4274	CD1	LEU	B	350	17.767	89.594	35.977	1.00	25.14	B	C
ATOM	4275	CD2	LEU	B	350	16.518	88.116	34.368	1.00	24.46	B	C
ATOM	4276	C	LEU	B	350	15.368	88.002	39.157	1.00	44.38	B	C
ATOM	4277	O	LEU	B	350	14.371	88.673	38.936	1.00	46.35	B	O
ATOM	4278	N	ILE	B	351	15.477	87.233	40.227	1.00	13.37	B	N
ATOM	4279	CA	ILE	B	351	14.406	87.183	41.217	1.00	14.30	B	C
ATOM	4280	CB	ILE	B	351	14.625	86.028	42.207	1.00	30.71	B	C
ATOM	4281	CG2	ILE	B	351	13.679	86.145	43.373	1.00	30.08	B	C
ATOM	4282	CG1	ILE	B	351	14.431	84.693	41.495	1.00	28.97	B	C
ATOM	4283	CD1	ILE	B	351	14.916	83.526	42.294	1.00	30.07	B	C
ATOM	4284	C	ILE	B	351	14.425	88.494	41.991	1.00	15.59	B	C
ATOM	4285	O	ILE	B	351	15.487	88.923	42.456	1.00	16.56	B	O
ATOM	4286	N	LYS	B	352	13.272	89.144	42.145	1.00	51.75	B	N
ATOM	4287	CA	LYS	B	352	13.264	90.416	42.865	1.00	52.19	B	C
ATOM	4288	CB	LYS	B	352	11.888	91.091	42.798	1.00	41.79	B	C
ATOM	4289	CG	LYS	B	352	11.610	91.809	41.466	1.00	42.10	B	C
ATOM	4290	CD	LYS	B	352	10.431	92.768	41.592	1.00	39.85	B	C
ATOM	4291	CE	LYS	B	352	10.068	93.440	40.270	1.00	38.73	B	C
ATOM	4292	NZ	LYS	B	352	9.404	92.544	39.273	1.00	39.11	B	N
ATOM	4293	C	LYS	B	352	13.735	90.291	44.310	1.00	53.08	B	C
ATOM	4294	O	LYS	B	352	14.913	90.488	44.581	1.00	54.11	B	O

ATOM	4295	N	ASN	B	353	12.842	89.956	45.234	1.00	37.53	B	N
ATOM	4296	CA	ASN	B	353	13.232	89.824	46.641	1.00	38.47	B	C
ATOM	4297	CB	ASN	B	353	12.178	89.041	47.421	1.00	67.53	B	C
ATOM	4298	CG	ASN	B	353	12.693	88.563	48.763	1.00	66.08	B	C
ATOM	4299	OD1	ASN	B	353	13.588	89.170	49.357	1.00	62.28	B	O
ATOM	4300	ND2	ASN	B	353	12.125	87.475	49.255	1.00	68.63	B	N
ATOM	4301	C	ASN	B	353	14.600	89.182	46.870	1.00	37.92	B	C
ATOM	4302	O	ASN	B	353	14.803	87.998	46.632	1.00	37.28	B	O
ATOM	4303	N	PRO	B	354	15.555	89.968	47.363	1.00	42.19	B	N
ATOM	4304	CD	PRO	B	354	15.431	91.386	47.729	1.00	60.71	B	C
ATOM	4305	CA	PRO	B	354	16.905	89.491	47.623	1.00	41.81	B	C
ATOM	4306	CB	PRO	B	354	17.506	90.625	48.434	1.00	60.98	B	C
ATOM	4307	CG	PRO	B	354	16.878	91.813	47.803	1.00	61.80	B	C
ATOM	4308	C	PRO	B	354	16.985	88.160	48.340	1.00	41.46	B	C
ATOM	4309	O	PRO	B	354	17.850	87.348	48.034	1.00	40.84	B	O
ATOM	4310	N	ALA	B	355	16.095	87.929	49.295	1.00	32.37	B	N
ATOM	4311	CA	ALA	B	355	16.136	86.681	50.035	1.00	34.42	B	C
ATOM	4312	CB	ALA	B	355	15.018	86.616	50.996	1.00	8.24	B	C
ATOM	4313	C	ALA	B	355	16.036	85.526	49.079	1.00	34.16	B	C
ATOM	4314	O	ALA	B	355	16.922	84.675	49.031	1.00	33.67	B	O
ATOM	4315	N	GLU	B	356	14.949	85.511	48.315	1.00	25.86	B	N
ATOM	4316	CA	GLU	B	356	14.681	84.459	47.341	1.00	26.90	B	C
ATOM	4317	CB	GLU	B	356	13.304	84.704	46.734	1.00	75.50	B	C
ATOM	4318	CG	GLU	B	356	12.230	84.627	47.799	1.00	82.25	B	C
ATOM	4319	CD	GLU	B	356	10.907	85.212	47.376	1.00	85.04	B	C
ATOM	4320	OE1	GLU	B	356	10.379	84.800	46.319	1.00	86.11	B	O
ATOM	4321	OE2	GLU	B	356	10.389	86.079	48.114	1.00	85.07	B	O
ATOM	4322	C	GLU	B	356	15.750	84.312	46.251	1.00	26.54	B	C
ATOM	4323	O	GLU	B	356	16.184	83.198	45.940	1.00	25.22	B	O
ATOM	4324	N	ARG	B	357	16.179	85.435	45.684	1.00	34.12	B	N
ATOM	4325	CA	ARG	B	357	17.196	85.430	44.642	1.00	32.33	B	C
ATOM	4326	CB	ARG	B	357	17.671	86.857	44.385	1.00	47.51	B	C
ATOM	4327	CG	ARG	B	357	17.949	87.188	42.928	1.00	42.82	B	C
ATOM	4328	CD	ARG	B	357	18.457	88.619	42.794	1.00	41.97	B	C
ATOM	4329	NE	ARG	B	357	17.620	89.570	43.522	1.00	39.82	B	N
ATOM	4330	CZ	ARG	B	357	18.016	90.787	43.874	1.00	38.06	B	C
ATOM	4331	NH1	ARG	B	357	19.232	91.200	43.559	1.00	37.03	B	N
ATOM	4332	NH2	ARG	B	357	17.215	91.578	44.572	1.00	37.10	B	N
ATOM	4333	C	ARG	B	357	18.379	84.562	45.067	1.00	31.56	B	C
ATOM	4334	O	ARG	B	357	18.711	84.481	46.253	1.00	31.93	B	O
ATOM	4335	N	ALA	B	358	19.007	83.908	44.094	1.00	30.00	B	N
ATOM	4336	CA	ALA	B	358	20.155	83.049	44.361	1.00	29.69	B	C
ATOM	4337	CB	ALA	B	358	20.546	82.298	43.115	1.00	38.42	B	C

ATOM	4338	C	ALA	B	358	21.322	83.880	44.843	1.00	30.17	B	C
ATOM	4339	O	ALA	B	358	21.454	85.045	44.475	1.00	31.07	B	O
ATOM	4340	N	ASP	B	359	22.178	83.278	45.660	1.00	16.21	B	N
ATOM	4341	CA	ASP	B	359	23.336	83.979	46.208	1.00	16.34	B	C
ATOM	4342	CB	ASP	B	359	23.407	83.790	47.711	1.00	54.40	B	C
ATOM	4343	CG	ASP	B	359	24.115	82.527	48.087	1.00	53.76	B	C
ATOM	4344	OD1	ASP	B	359	23.844	81.492	47.447	1.00	49.92	B	O
ATOM	4345	OD2	ASP	B	359	24.941	82.570	49.018	1.00	54.94	B	O
ATOM	4346	C	ASP	B	359	24.601	83.435	45.590	1.00	15.91	B	C
ATOM	4347	O	ASP	B	359	24.621	82.318	45.104	1.00	14.27	B	O
ATOM	4348	N	LEU	B	360	25.661	84.230	45.636	1.00	43.28	B	N
ATOM	4349	CA	LEU	B	360	26.944	83.859	45.054	1.00	41.33	B	C
ATOM	4350	CB	LEU	B	360	28.075	84.600	45.758	1.00	17.18	B	C
ATOM	4351	CG	LEU	B	360	29.096	85.257	44.831	1.00	15.93	B	C
ATOM	4352	CD1	LEU	B	360	28.370	86.068	43.798	1.00	14.60	B	C
ATOM	4353	CD2	LEU	B	360	30.034	86.158	45.619	1.00	16.78	B	C
ATOM	4354	C	LEU	B	360	27.236	82.375	45.063	1.00	40.00	B	C
ATOM	4355	O	LEU	B	360	27.576	81.813	44.028	1.00	39.63	B	O
ATOM	4356	N	LYS	B	361	27.096	81.736	46.220	1.00	36.43	B	N
ATOM	4357	CA	LYS	B	361	27.379	80.308	46.320	1.00	39.15	B	C
ATOM	4358	CB	LYS	B	361	27.270	79.834	47.770	1.00	126.40	B	C
ATOM	4359	CG	LYS	B	361	27.610	78.361	47.961	1.00	125.34	B	C
ATOM	4360	CD	LYS	B	361	27.616	77.976	49.436	1.00	124.52	B	C
ATOM	4361	CE	LYS	B	361	27.607	76.457	49.643	1.00	123.41	B	C
ATOM	4362	NZ	LYS	B	361	28.810	75.745	49.122	1.00	126.38	B	N
ATOM	4363	C	LYS	B	361	26.451	79.495	45.436	1.00	40.58	B	C
ATOM	4364	O	LYS	B	361	26.902	78.823	44.506	1.00	40.54	B	O
ATOM	4365	N	MET	B	362	25.156	79.557	45.728	1.00	22.71	B	N
ATOM	4366	CA	MET	B	362	24.162	78.831	44.946	1.00	23.77	B	C
ATOM	4367	CB	MET	B	362	22.763	79.406	45.223	1.00	80.07	B	C
ATOM	4368	CG	MET	B	362	21.736	79.219	44.096	1.00	85.17	B	C
ATOM	4369	SD	MET	B	362	20.911	77.606	43.946	1.00	91.12	B	S
ATOM	4370	CE	MET	B	362	19.331	77.957	44.738	1.00	90.93	B	C
ATOM	4371	C	MET	B	362	24.495	78.915	43.453	1.00	22.71	B	C
ATOM	4372	O	MET	B	362	24.409	77.931	42.725	1.00	22.68	B	O
ATOM	4373	N	LEU	B	363	24.903	80.091	43.003	1.00	33.99	B	N
ATOM	4374	CA	LEU	B	363	25.226	80.275	41.601	1.00	33.76	B	C
ATOM	4375	CB	LEU	B	363	25.404	81.757	41.295	1.00	27.39	B	C
ATOM	4376	CG	LEU	B	363	24.093	82.524	41.419	1.00	26.70	B	C
ATOM	4377	CD1	LEU	B	363	24.280	83.903	40.867	1.00	26.71	B	C
ATOM	4378	CD2	LEU	B	363	23.005	81.802	40.661	1.00	24.11	B	C
ATOM	4379	C	LEU	B	363	26.450	79.506	41.164	1.00	32.69	B	C
ATOM	4380	O	LEU	B	363	26.441	78.886	40.111	1.00	33.14	B	O

ATOM	4381	N	THR	B	364	27.507	79.542	41.965	1.00	62.52	B	N
ATOM	4382	CA	THR	B	364	28.724	78.823	41.612	1.00	63.10	B	C
ATOM	4383	CB	THR	B	364	29.860	79.129	42.596	1.00	44.87	B	C
ATOM	4384	OG1	THR	B	364	30.474	80.376	42.243	1.00	43.78	B	O
ATOM	4385	CG2	THR	B	364	30.898	78.042	42.556	1.00	46.65	B	C
ATOM	4386	C	THR	B	364	28.482	77.319	41.568	1.00	62.61	B	C
ATOM	4387	O	THR	B	364	29.166	76.590	40.850	1.00	63.38	B	O
ATOM	4388	N	ASN	B	365	27.496	76.860	42.328	1.00	36.61	B	N
ATOM	4389	CA	ASN	B	365	27.172	75.444	42.355	1.00	35.46	B	C
ATOM	4390	CB	ASN	B	365	26.434	75.089	43.645	1.00	106.63	B	C
ATOM	4391	CG	ASN	B	365	27.312	75.231	44.877	1.00	109.40	B	C
ATOM	4392	OD1	ASN	B	365	26.854	75.058	46.011	1.00	113.65	B	O
ATOM	4393	ND2	ASN	B	365	28.585	75.544	44.659	1.00	110.84	B	N
ATOM	4394	C	ASN	B	365	26.319	75.096	41.155	1.00	34.14	B	C
ATOM	4395	O	ASN	B	365	26.641	74.190	40.417	1.00	35.18	B	O
ATOM	4396	N	HIS	B	366	25.238	75.831	40.952	1.00	46.41	B	N
ATOM	4397	CA	HIS	B	366	24.331	75.588	39.828	1.00	45.21	B	C
ATOM	4398	CB	HIS	B	366	23.751	76.914	39.348	1.00	72.79	B	C
ATOM	4399	CG	HIS	B	366	22.501	76.764	38.547	1.00	72.09	B	C
ATOM	4400	CD2	HIS	B	366	22.310	76.583	37.220	1.00	71.37	B	C
ATOM	4401	ND1	HIS	B	366	21.250	76.750	39.121	1.00	73.51	B	N
ATOM	4402	CE1	HIS	B	366	20.340	76.567	38.181	1.00	73.69	B	C
ATOM	4403	NE2	HIS	B	366	20.957	76.462	37.019	1.00	73.03	B	N
ATOM	4404	C	HIS	B	366	24.979	74.865	38.639	1.00	42.74	B	C
ATOM	4405	O	HIS	B	366	26.050	75.257	38.174	1.00	41.57	B	O
ATOM	4406	N	THR	B	367	24.313	73.826	38.138	1.00	29.64	B	N
ATOM	4407	CA	THR	B	367	24.838	73.045	37.021	1.00	29.64	B	C
ATOM	4408	CB	THR	B	367	23.820	72.006	36.517	1.00	27.70	B	C
ATOM	4409	OG1	THR	B	367	22.668	72.665	36.002	1.00	28.70	B	O
ATOM	4410	CG2	THR	B	367	23.399	71.102	37.632	1.00	28.77	B	C
ATOM	4411	C	THR	B	367	25.299	73.844	35.810	1.00	28.49	B	C
ATOM	4412	O	THR	B	367	26.273	73.474	35.147	1.00	29.15	B	O
ATOM	4413	N	PHE	B	368	24.600	74.929	35.505	1.00	27.61	B	N
ATOM	4414	CA	PHE	B	368	24.960	75.740	34.357	1.00	28.18	B	C
ATOM	4415	CB	PHE	B	368	24.097	76.991	34.287	1.00	39.85	B	C
ATOM	4416	CG	PHE	B	368	24.544	77.963	33.244	1.00	37.40	B	C
ATOM	4417	CD1	PHE	B	368	24.309	77.718	31.903	1.00	37.51	B	C
ATOM	4418	CD2	PHE	B	368	25.246	79.096	33.596	1.00	36.60	B	C
ATOM	4419	CE1	PHE	B	368	24.768	78.582	30.928	1.00	37.85	B	C
ATOM	4420	CE2	PHE	B	368	25.709	79.967	32.624	1.00	36.60	B	C
ATOM	4421	CZ	PHE	B	368	25.468	79.705	31.286	1.00	36.60	B	C
ATOM	4422	C	PHE	B	368	26.411	76.166	34.419	1.00	27.27	B	C
ATOM	4423	O	PHE	B	368	27.161	75.992	33.452	1.00	25.08	B	O

ATOM	4424	N	ILE	B	369	26.802	76.729	35.563	1.00	29.32	B N
ATOM	4425	CA	ILE	B	369	28.165	77.215	35.758	1.00	34.22	B C
ATOM	4426	CB	ILE	B	369	28.333	77.983	37.074	1.00	20.96	B C
ATOM	4427	CG2	ILE	B	369	29.775	78.388	37.236	1.00	19.59	B C
ATOM	4428	CG1	ILE	B	369	27.489	79.255	37.049	1.00	20.84	B C
ATOM	4429	CD1	ILE	B	369	27.749	80.132	35.835	1.00	22.82	B C
ATOM	4430	C	ILE	B	369	29.181	76.108	35.746	1.00	36.60	B C
ATOM	4431	O	ILE	B	369	30.275	76.269	35.222	1.00	37.41	B O
ATOM	4432	N	LYS	B	370	28.828	74.981	36.341	1.00	49.56	B N
ATOM	4433	CA	LYS	B	370	29.752	73.867	36.351	1.00	51.50	B C
ATOM	4434	CB	LYS	B	370	29.259	72.780	37.300	1.00	27.51	B C
ATOM	4435	CG	LYS	B	370	29.404	73.200	38.747	1.00	30.45	B C
ATOM	4436	CD	LYS	B	370	28.928	72.120	39.660	1.00	35.13	B C
ATOM	4437	CE	LYS	B	370	27.551	71.640	39.242	1.00	36.85	B C
ATOM	4438	NZ	LYS	B	370	27.086	70.519	40.114	1.00	37.81	B N
ATOM	4439	C	LYS	B	370	29.869	73.380	34.919	1.00	51.41	B C
ATOM	4440	O	LYS	B	370	30.974	73.270	34.387	1.00	49.93	B O
ATOM	4441	N	ARG	B	371	28.732	73.114	34.286	1.00	26.13	B N
ATOM	4442	CA	ARG	B	371	28.748	72.698	32.899	1.00	26.05	B C
ATOM	4443	CB	ARG	B	371	27.343	72.814	32.314	1.00	43.39	B C
ATOM	4444	CG	ARG	B	371	27.164	72.123	30.982	1.00	43.04	B C
ATOM	4445	CD	ARG	B	371	25.931	72.620	30.289	1.00	43.16	B C
ATOM	4446	NE	ARG	B	371	26.096	74.025	29.953	1.00	42.39	B N
ATOM	4447	CZ	ARG	B	371	25.174	74.772	29.357	1.00	40.44	B C
ATOM	4448	NH1	ARG	B	371	24.002	74.254	29.019	1.00	38.89	B N
ATOM	4449	NH2	ARG	B	371	25.426	76.047	29.106	1.00	39.16	B N
ATOM	4450	C	ARG	B	371	29.702	73.666	32.165	1.00	25.45	B C
ATOM	4451	O	ARG	B	371	30.499	73.279	31.316	1.00	25.58	B O
ATOM	4452	N	SER	B	372	29.637	74.938	32.524	1.00	36.48	B N
ATOM	4453	CA	SER	B	372	30.478	75.936	31.886	1.00	39.83	B C
ATOM	4454	CB	SER	B	372	29.993	77.339	32.260	1.00	124.79	B C
ATOM	4455	OG	SER	B	372	28.642	77.536	31.883	1.00	125.57	B O
ATOM	4456	C	SER	B	372	31.949	75.804	32.245	1.00	41.87	B C
ATOM	4457	O	SER	B	372	32.813	76.160	31.457	1.00	42.12	B O
ATOM	4458	N	GLU	B	373	32.240	75.297	33.435	1.00	35.21	B N
ATOM	4459	CA	GLU	B	373	33.624	75.176	33.866	1.00	36.20	B C
ATOM	4460	CB	GLU	B	373	33.679	74.854	35.357	1.00	90.65	B C
ATOM	4461	CG	GLU	B	373	33.393	76.061	36.232	1.00	94.87	B C
ATOM	4462	CD	GLU	B	373	33.450	75.734	37.702	1.00	97.65	B C
ATOM	4463	OE1	GLU	B	373	33.406	76.675	38.523	1.00	99.69	B O
ATOM	4464	OE2	GLU	B	373	33.535	74.531	38.031	1.00	97.56	B O
ATOM	4465	C	GLU	B	373	34.420	74.158	33.062	1.00	36.00	B C
ATOM	4466	O	GLU	B	373	35.600	73.903	33.332	1.00	35.29	B O

ATOM	4467	N	VAL	B	374	33.770	73.596	32.049	1.00 78.11	B	N
ATOM	4468	CA	VAL	B	374	34.401	72.611	31.185	1.00 79.20	B	C
ATOM	4469	CB	VAL	B	374	34.044	71.181	31.645	1.00 42.85	B	C
ATOM	4470	CG1	VAL	B	374	34.153	71.070	33.156	1.00 42.24	B	C
ATOM	4471	CG2	VAL	B	374	32.644	70.830	31.193	1.00 41.37	B	C
ATOM	4472	C	VAL	B	374	33.922	72.820	29.742	1.00 78.12	B	C
ATOM	4473	O	VAL	B	374	32.890	73.452	29.508	1.00 79.70	B	O
ATOM	4474	N	GLU	B	375	34.690	72.294	28.791	1.00131.24	B	N
ATOM	4475	CA	GLU	B	375	34.391	72.384	27.360	1.00131.37	B	C
ATOM	4476	CB	GLU	B	375	32.894	72.644	27.126	1.00108.91	B	C
ATOM	4477	CG	GLU	B	375	32.495	72.737	25.653	1.00102.93	B	C
ATOM	4478	CD	GLU	B	375	32.649	71.419	24.906	1.00 97.65	B	C
ATOM	4479	OE1	GLU	B	375	31.663	70.654	24.842	1.00 98.01	B	O
ATOM	4480	OE2	GLU	B	375	33.755	71.146	24.392	1.00 96.01	B	O
ATOM	4481	C	GLU	B	375	35.223	73.439	26.613	1.00133.00	B	C
ATOM	4482	O	GLU	B	375	35.868	74.296	27.221	1.00133.37	B	O
ATOM	4483	N	GLU	B	376	35.189	73.342	25.286	1.00102.49	B	N
ATOM	4484	CA	GLU	B	376	35.898	74.217	24.353	1.00105.24	B	C
ATOM	4485	CB	GLU	B	376	35.441	73.876	22.929	1.00203.67	B	C
ATOM	4486	CG	GLU	B	376	36.186	74.587	21.814	1.00203.67	B	C
ATOM	4487	CD	GLU	B	376	35.698	74.162	20.441	1.00203.67	B	C
ATOM	4488	OE1	GLU	B	376	34.525	74.442	20.113	1.00203.67	B	O
ATOM	4489	OE2	GLU	B	376	36.484	73.542	19.693	1.00203.67	B	O
ATOM	4490	C	GLU	B	376	35.757	75.729	24.582	1.00106.34	B	C
ATOM	4491	O	GLU	B	376	34.737	76.332	24.236	1.00108.15	B	O
ATOM	4492	N	VAL	B	377	36.794	76.335	25.155	1.00130.02	B	N
ATOM	4493	CA	VAL	B	377	36.807	77.775	25.410	1.00131.93	B	C
ATOM	4494	CB	VAL	B	377	38.066	78.210	26.241	1.00 88.03	B	C
ATOM	4495	CG1	VAL	B	377	37.829	77.994	27.724	1.00 87.33	B	C
ATOM	4496	CG2	VAL	B	377	39.291	77.408	25.802	1.00 86.83	B	C
ATOM	4497	C	VAL	B	377	36.844	78.505	24.070	1.00132.37	B	C
ATOM	4498	O	VAL	B	377	35.863	78.530	23.325	1.00132.05	B	O
ATOM	4499	N	ASP	B	378	38.007	79.085	23.789	1.00143.23	B	N
ATOM	4500	CA	ASP	B	378	38.285	79.824	22.565	1.00143.63	B	C
ATOM	4501	CB	ASP	B	378	37.755	79.078	21.339	1.00 82.02	B	C
ATOM	4502	CG	ASP	B	378	38.601	79.330	20.103	1.00 79.09	B	C
ATOM	4503	OD1	ASP	B	378	38.182	78.932	18.993	1.00 77.88	B	O
ATOM	4504	OD2	ASP	B	378	39.695	79.921	20.248	1.00 76.46	B	O
ATOM	4505	C	ASP	B	378	37.719	81.232	22.596	1.00145.38	B	C
ATOM	4506	O	ASP	B	378	37.555	81.863	21.552	1.00147.42	B	O
ATOM	4507	N	PHE	B	379	37.415	81.720	23.794	1.00 64.54	B	N
ATOM	4508	CA	PHE	B	379	36.897	83.069	23.933	1.00 63.51	B	C
ATOM	4509	CB	PHE	B	379	36.921	83.492	25.404	1.00 58.72	B	C

ATOM	4510	CG	PHE	B	379	36.389	84.877	25.646	1.00	57.84	B	C
ATOM	4511	CD1	PHE	B	379	37.226	85.889	26.083	1.00	58.39	B	C
ATOM	4512	CD2	PHE	B	379	35.060	85.174	25.392	1.00	56.28	B	C
ATOM	4513	CE1	PHE	B	379	36.750	87.174	26.259	1.00	57.89	B	C
ATOM	4514	CE2	PHE	B	379	34.581	86.456	25.565	1.00	55.26	B	C
ATOM	4515	CZ	PHE	B	379	35.430	87.459	25.999	1.00	55.97	B	C
ATOM	4516	C	PHE	B	379	37.824	83.953	23.095	1.00	63.21	B	C
ATOM	4517	O	PHE	B	379	37.378	84.792	22.312	1.00	63.68	B	O
ATOM	4518	N	ALA	B	380	39.123	83.743	23.253	1.00	46.86	B	N
ATOM	4519	CA	ALA	B	380	40.103	84.498	22.493	1.00	48.61	B	C
ATOM	4520	CB	ALA	B	380	41.501	84.071	22.890	1.00	98.14	B	C
ATOM	4521	C	ALA	B	380	39.876	84.243	21.000	1.00	49.06	B	C
ATOM	4522	O	ALA	B	380	39.980	85.153	20.172	1.00	47.63	B	O
ATOM	4523	N	GLY	B	381	39.565	82.995	20.666	1.00	87.24	B	N
ATOM	4524	CA	GLY	B	381	39.329	82.642	19.281	1.00	89.07	B	C
ATOM	4525	C	GLY	B	381	38.164	83.417	18.708	1.00	90.95	B	C
ATOM	4526	O	GLY	B	381	38.305	84.120	17.713	1.00	91.76	B	O
ATOM	4527	N	TRP	B	382	37.010	83.285	19.347	1.00	54.45	B	N
ATOM	4528	CA	TRP	B	382	35.787	83.970	18.930	1.00	53.56	B	C
ATOM	4529	CB	TRP	B	382	34.633	83.509	19.827	1.00	64.53	B	C
ATOM	4530	CG	TRP	B	382	33.372	84.334	19.753	1.00	64.49	B	C
ATOM	4531	CD2	TRP	B	382	33.071	85.520	20.506	1.00	64.46	B	C
ATOM	4532	CE2	TRP	B	382	31.774	85.930	20.139	1.00	65.19	B	C
ATOM	4533	CE3	TRP	B	382	33.773	86.275	21.447	1.00	64.11	B	C
ATOM	4534	CD1	TRP	B	382	32.272	84.083	18.984	1.00	65.32	B	C
ATOM	4535	NE1	TRP	B	382	31.305	85.035	19.213	1.00	65.30	B	N
ATOM	4536	CZ2	TRP	B	382	31.166	87.055	20.686	1.00	64.93	B	C
ATOM	4537	CZ3	TRP	B	382	33.167	87.393	21.986	1.00	64.95	B	C
ATOM	4538	CH2	TRP	B	382	31.879	87.773	21.603	1.00	65.40	B	C
ATOM	4539	C	TRP	B	382	35.908	85.501	18.992	1.00	53.61	B	C
ATOM	4540	O	TRP	B	382	35.558	86.198	18.035	1.00	53.98	B	O
ATOM	4541	N	LEU	B	383	36.407	86.013	20.117	1.00	80.70	B	N
ATOM	4542	CA	LEU	B	383	36.544	87.451	20.317	1.00	83.14	B	C
ATOM	4543	CB	LEU	B	383	37.109	87.738	21.707	1.00	35.96	B	C
ATOM	4544	CG	LEU	B	383	37.200	89.222	22.085	1.00	36.12	B	C
ATOM	4545	CD1	LEU	B	383	35.821	89.793	22.344	1.00	36.13	B	C
ATOM	4546	CD2	LEU	B	383	38.055	89.375	23.321	1.00	34.79	B	C
ATOM	4547	C	LEU	B	383	37.406	88.122	19.258	1.00	84.52	B	C
ATOM	4548	O	LEU	B	383	37.096	89.223	18.806	1.00	83.05	B	O
ATOM	4549	N	CYS	B	384	38.487	87.467	18.856	1.00	73.09	B	N
ATOM	4550	CA	CYS	B	384	39.356	88.036	17.837	1.00	73.95	B	C
ATOM	4551	CB	CYS	B	384	40.690	87.298	17.813	1.00	97.24	B	C
ATOM	4552	SG	CYS	B	384	41.630	87.562	19.319	1.00	99.10	B	S

ATOM	4553	C	CYS	B	384	38.691	87.988	16.466	1.00 75.45	B	C
ATOM	4554	O	CYS	B	384	38.771	88.954	15.706	1.00 75.00	B	O
ATOM	4555	N	LYS	B	385	38.037	86.868	16.154	1.00 79.71	B	N
ATOM	4556	CA	LYS	B	385	37.339	86.722	14.877	1.00 80.74	B	C
ATOM	4557	CB	LYS	B	385	36.368	85.537	14.907	1.00108.91	B	C
ATOM	4558	CG	LYS	B	385	36.979	84.156	14.731	1.00111.35	B	C
ATOM	4559	CD	LYS	B	385	35.878	83.094	14.753	1.00113.91	B	C
ATOM	4560	CE	LYS	B	385	36.414	81.694	14.483	1.00115.04	B	C
ATOM	4561	NZ	LYS	B	385	35.324	80.675	14.524	1.00115.50	B	N
ATOM	4562	C	LYS	B	385	36.524	87.987	14.685	1.00 79.15	B	C
ATOM	4563	O	LYS	B	385	36.425	88.532	13.581	1.00 79.17	B	O
ATOM	4564	N	THR	B	386	35.942	88.435	15.793	1.00106.27	B	N
ATOM	4565	CA	THR	B	386	35.106	89.622	15.834	1.00107.39	B	C
ATOM	4566	CB	THR	B	386	34.185	89.586	17.076	1.00 62.12	B	C
ATOM	4567	OG1	THR	B	386	33.219	88.538	16.925	1.00 61.07	B	O
ATOM	4568	CG2	THR	B	386	33.458	90.911	17.251	1.00 61.98	B	C
ATOM	4569	C	THR	B	386	35.918	90.912	15.850	1.00108.64	B	C
ATOM	4570	O	THR	B	386	36.320	91.415	14.800	1.00108.97	B	O
ATOM	4571	N	LEU	B	387	36.160	91.434	17.048	1.00 70.69	B	N
ATOM	4572	CA	LEU	B	387	36.903	92.675	17.231	1.00 70.26	B	C
ATOM	4573	CB	LEU	B	387	37.358	92.806	18.688	1.00106.87	B	C
ATOM	4574	CG	LEU	B	387	36.314	92.478	19.755	1.00103.34	B	C
ATOM	4575	CD1	LEU	B	387	36.813	92.936	21.119	1.00101.44	B	C
ATOM	4576	CD2	LEU	B	387	35.003	93.158	19.402	1.00101.67	B	C
ATOM	4577	C	LEU	B	387	38.120	92.817	16.315	1.00 72.68	B	C
ATOM	4578	O	LEU	B	387	38.692	93.905	16.209	1.00 73.99	B	O
ATOM	4579	N	ARG	B	388	38.516	91.721	15.671	1.00 90.93	B	N
ATOM	4580	CA	ARG	B	388	39.663	91.716	14.764	1.00 92.67	B	C
ATOM	4581	CB	ARG	B	388	39.250	92.266	13.401	1.00119.06	B	C
ATOM	4582	CG	ARG	B	388	38.480	91.255	12.583	1.00120.28	B	C
ATOM	4583	CD	ARG	B	388	39.063	89.860	12.813	1.00121.80	B	C
ATOM	4584	NE	ARG	B	388	38.777	88.926	11.726	1.00124.61	B	N
ATOM	4585	CZ	ARG	B	388	39.380	88.947	10.539	1.00125.62	B	C
ATOM	4586	NH1	ARG	B	388	40.311	89.855	10.274	1.00126.19	B	N
ATOM	4587	NH2	ARG	B	388	39.050	88.061	9.611	1.00126.07	B	N
ATOM	4588	C	ARG	B	388	40.891	92.466	15.286	1.00 92.38	B	C
ATOM	4589	O	ARG	B	388	41.135	93.625	14.933	1.00 91.92	B	O
ATOM	4590	N	LEU	B	389	41.675	91.778	16.111	1.00149.52	B	N
ATOM	4591	CA	LEU	B	389	42.868	92.366	16.702	1.00150.84	B	C
ATOM	4592	CB	LEU	B	389	42.774	92.277	18.230	1.00 70.18	B	C
ATOM	4593	CG	LEU	B	389	41.412	92.638	18.840	1.00 71.21	B	C
ATOM	4594	CD1	LEU	B	389	41.489	92.607	20.353	1.00 70.55	B	C
ATOM	4595	CD2	LEU	B	389	40.988	94.013	18.371	1.00 71.86	B	C

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ATOM   4596  C   LEU B 389     44.152  91.689  16.213  1.00151.61      B    C
ATOM   4597  O   LEU B 389     44.194  90.469  16.032  1.00150.15      B    O
ATOM   4598  N   ASN B 390     45.191  92.495  15.998  1.00203.67      B    N
ATOM   4599  CA  ASN B 390     46.488  92.002  15.534  1.00203.67      B    C
ATOM   4600  CB  ASN B 390     46.876  92.661  14.208  1.00106.37      B    C
ATOM   4601  CG  ASN B 390     45.953  92.279  13.077  1.00106.60      B    C
ATOM   4602  OD1 ASN B 390     44.760  92.589  13.101  1.00106.59      B    O
ATOM   4603  ND2 ASN B 390     46.500  91.597  12.074  1.00106.22      B    N
ATOM   4604  C   ASN B 390     47.590  92.282  16.547  1.00203.67      B    C
ATOM   4605  O   ASN B 390     47.390  92.155  17.757  1.00203.67      B    O
ATOM   4606  N   GLN B 391     48.753  92.667  16.031  1.00168.93      B    N
ATOM   4607  CA  GLN B 391     49.911  92.978  16.858  1.00170.58      B    C
ATOM   4608  CB  GLN B 391     50.203  91.827  17.822  1.00184.34      B    C
ATOM   4609  CG  GLN B 391     51.060  92.214  19.019  1.00185.89      B    C
ATOM   4610  CD  GLN B 391     50.353  93.178  19.957  1.00186.81      B    C
ATOM   4611  OE1 GLN B 391     50.875  93.527  21.017  1.00187.00      B    O
ATOM   4612  NE2 GLN B 391     49.159  93.614  19.571  1.00187.22      B    N
ATOM   4613  C   GLN B 391     51.124  93.216  15.964  1.00170.59      B    C
ATOM   4614  O   GLN B 391     50.951  93.201  14.726  1.00170.81      B    O
ATOM   4615  OXT GLN B 391     52.229  93.414  16.513  1.00184.22      B    O
TER    4616      GLN B 391                                              B
ATOM   4617  PG  ATP C   1     23.028 120.762  36.245  1.00 24.10      CMEK P
ATOM   4618  O1G ATP C   1     22.221 120.220  37.473  1.00 25.10      CMEK O
ATOM   4619  O2G ATP C   1     22.236 121.899  35.706  1.00 26.10      CMEK O
ATOM   4620  O3G ATP C   1     23.194 119.741  35.266  1.00 27.10      CMEK O
ATOM   4621  PB  ATP C   1     25.001 121.491  38.099  1.00 28.10      CMEK P
ATOM   4622  O1B ATP C   1     24.082 122.360  38.753  1.00 29.10      CMEK O
ATOM   4623  O2B ATP C   1     25.120 120.387  38.991  1.00 30.10      CMEK O
ATOM   4624  O3B ATP C   1     24.401 121.382  36.763  1.00 31.10      CMEK O
ATOM   4625  PA  ATP C   1     27.234 122.379  36.725  1.00 32.10      CMEK P
ATOM   4626  O1A ATP C   1     28.194 121.216  36.635  1.00 33.10      CMEK O
ATOM   4627  O2A ATP C   1     26.352 122.674  35.497  1.00 34.10      CMEK O
ATOM   4628  O3A ATP C   1     26.350 122.197  37.938  1.00 35.10      CMEK O
ATOM   4629  O5' ATP C   1     27.940 123.698  37.398  1.00 36.10      CMEK O
ATOM   4630  C5' ATP C   1     28.772 123.422  38.569  1.00 37.10      CMEK C
ATOM   4631  C4' ATP C   1     28.635 124.391  39.572  1.00 38.10      CMEK C
ATOM   4632  O4' ATP C   1     29.558 125.469  39.261  1.00 39.10      CMEK O
ATOM   4633  C3' ATP C   1     27.269 125.124  39.707  1.00 40.10      CMEK C
ATOM   4634  O3' ATP C   1     26.294 124.380  40.464  1.00 41.10      CMEK O
ATOM   4635  C2' ATP C   1     27.717 126.449  40.303  1.00 42.10      CMEK C
ATOM   4636  O2' ATP C   1     27.812 126.351  41.745  1.00 43.10      CMEK O
ATOM   4637  C1' ATP C   1     29.028 126.711  39.681  1.00 44.10      CMEK C
ATOM   4638  N9  ATP C   1     28.927 127.636  38.517  1.00 45.10      CMEK N
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ATOM   4639  C8  ATP C   1      28.311 127.466  37.245  1.00 46.10      CMEK C
ATOM   4640  N7  ATP C   1      28.418 128.541  36.433  1.00 47.10      CMEK N
ATOM   4641  C5  ATP C   1      29.163 129.408  37.317  1.00 48.10      CMEK C
ATOM   4642  C6  ATP C   1      29.577 130.748  36.974  1.00 49.10      CMEK C
ATOM   4643  N6  ATP C   1      29.349 131.405  35.809  1.00 50.10      CMEK N
ATOM   4644  N1  ATP C   1      30.306 131.446  37.980  1.00 51.10      CMEK N
ATOM   4645  C2  ATP C   1      30.574 130.793  39.242  1.00 52.10      CMEK C
ATOM   4646  N3  ATP C   1      30.199 129.561  39.585  1.00 53.10      CMEK N
ATOM   4647  C4  ATP C   1      29.470 128.901  38.536  1.00 54.10      CMEK C
TER    4648      ATP C   1                                              CMEK
ATOM   4649  PG  ATP D   2      29.424 104.838  32.878  1.00 75.15      DMEK P
ATOM   4650  O1G ATP D   2      28.163 104.521  32.044  1.00 75.28      DMEK O
ATOM   4651  O2G ATP D   2      29.347 103.988  34.063  1.00 76.99      DMEK O
ATOM   4652  O3G ATP D   2      29.463 106.193  33.255  1.00 80.23      DMEK O
ATOM   4653  PB  ATP D   2      31.113 103.262  31.222  1.00 66.58      DMEK P
ATOM   4654  O1B ATP D   2      31.019 102.134  32.097  1.00 73.34      DMEK O
ATOM   4655  O2B ATP D   2      30.363 102.866  30.062  1.00 72.36      DMEK O
ATOM   4656  O3B ATP D   2      30.725 104.378  32.109  1.00 76.32      DMEK O
ATOM   4657  PA  ATP D   2      33.650 104.372  31.504  1.00 70.83      DMEK P
ATOM   4658  O1A ATP D   2      33.308 105.811  31.297  1.00 74.45      DMEK O
ATOM   4659  O2A ATP D   2      33.895 103.914  32.924  1.00 72.07      DMEK O
ATOM   4660  O3A ATP D   2      32.592 103.498  30.869  1.00 72.74      DMEK O
ATOM   4661  O5' ATP D   2      34.778 103.860  30.457  1.00 68.35      DMEK O
ATOM   4662  C5' ATP D   2      34.611 104.240  29.065  1.00 68.49      DMEK C
ATOM   4663  C4' ATP D   2      34.664 103.110  28.238  1.00 71.78      DMEK C
ATOM   4664  O4' ATP D   2      36.063 102.830  27.928  1.00 69.78      DMEK O
ATOM   4665  C3' ATP D   2      34.162 101.779  28.829  1.00 71.02      DMEK C
ATOM   4666  O3' ATP D   2      32.729 101.656  28.752  1.00 73.14      DMEK O
ATOM   4667  C2' ATP D   2      34.989 100.779  28.035  1.00 68.97      DMEK C
ATOM   4668  O2' ATP D   2      34.314 100.473  26.803  1.00 71.55      DMEK O
ATOM   4669  C1' ATP D   2      36.286 101.443  27.803  1.00 66.97      DMEK C
ATOM   4670  N9  ATP D   2      37.345 101.058  28.772  1.00 65.61      DMEK N
ATOM   4671  C8  ATP D   2      37.527 101.449  30.122  1.00 62.14      DMEK C
ATOM   4672  N7  ATP D   2      38.613 100.910  30.717  1.00 65.57      DMEK N
ATOM   4673  C5  ATP D   2      39.112 100.134  29.616  1.00 64.85      DMEK C
ATOM   4674  C6  ATP D   2      40.304  99.324  29.690  1.00 65.51      DMEK C
ATOM   4675  N6  ATP D   2      41.103  99.177  30.755  1.00 62.71      DMEK N
ATOM   4676  N1  ATP D   2      40.666  98.612  28.510  1.00 64.42      DMEK N
ATOM   4677  C2  ATP D   2      39.825  98.745  27.334  1.00 63.10      DMEK C
ATOM   4678  N3  ATP D   2      38.702  99.501  27.238  1.00 65.01      DMEK N
ATOM   4679  C4  ATP D   2      38.393 100.195  28.467  1.00 66.09      DMEK C
TER    4680      ATP D   2                                              DMEK
ATOM   4681  C1  LIG P   1      23.850 126.521  29.116  1.00 35.58      LIG3 C
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ATOM   4682  C2  LIG P   1      25.029 127.180  29.556  1.00 35.58      LIG3 C
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Table 3

Multiple Sequence Alignment of Inhibitor-Binding Site Residues of MEK1 and MEK2 That are Within Either 4 Å or 5 Å of the MEK1 Inhibitor-Binding Site

Residues that are within 4 Å of the ligand		Residues that are within 5 Å of the ligand	
MEK1	Corresponding residues in MEK2	MEK1	Corresponding residues in MEK2
G77	G81	G77	G81
N78	N82	N78	N82
G79	G83	G79	G83
G80	G84	G80	G84
K97	K101	K97	K101
I99	I103	I99	I103
L115	L119	L115	L119
L118	L122	L118	L122
V127	V131	I126	I130
F129	F133	V127	V131
I141	I145	G128	G132
M143	M147	F129	F133

Table 3 (continued)

Multiple Sequence Alignment of Inhibitor-Binding Site Residues of MEK1 and MEK2 That are Within Either 4 Å or 5 Å of the MEK1 Inhibitor-Binding Site			
Residues that are within 4 Å of the ligand		Residues that are within 5 Å of the ligand	
MEK1	Corresponding residues in MEK2	MEK1	Corresponding residues in MEK2
C207	C211	I141	I145
D208	D212	M143	M147
F209	F213	D190	D194
G210	G214	N195	N199
V211	V215	L206	L210
S212	S216	C207	C211
L215	L219	D208	D212
I216	I220	F209	F213
M219	M223	G210	G214
		V211	V215
		S212	S216
		L215	L219
		I216	I220
		M219	M223
		F223	F227

Table 4

Multiple Sequence Alignment of Inibitor-Binding Site Residues of MEK1 and MEK2 That are Within Either 4 Å or 5 Å of the MEK1 Cofactor-Binding Site			
Residues that are within 4 Å of the ATP co-factor		**Residues that are within 5 Å of the ATP co-factor**	
MEK1	Corresponding residues in MEK2	MEK1	Corresponding residues in MEK2
L74	L78	L74	L78
G75	G79	G75	G79
A76	A80	A76	A80
G77	G81	G77	G81
N78	N82	N78	N82
G80	G84	G79	G83
V81	V85	G80	G84
V82	V86	V81	V85
A95	A99	V82	V86
K97	K101	A95	A99
V127	V131	K97	K101
M143	M147	V127	V131
E144	E148	M143	M147
H145	H149	E144	E148

Table 4 (continued)

Multiple Sequence Alignment of Inibitor-Binding Site Residues of MEK1 and MEK2 That are Within Either 4 Å or 5 Å of the MEK1 Cofactor-Binding Site			
Residues that are within 4 Å of the ATP co-factor		**Residues that are within 5 Å of the ATP co-factor**	
MEK1	Corresponding residues in MEK2	MEK1	Corresponding residues in MEK2
M146	M150	H145	H149
G149	G153	M146	M150
S150	S154	D147	D151
D152	D156	G149	G153
Q153	Q157	S150	S154
K192	K196	D152	D156
S194	S198	Q153	Q157
N195	N199	D190	D194
L197	L201	K192	K196
D208	D212	S194	S198
V224	V228	N195	N199
		L197	L201
		C207	C211
		D208	D212
		V224	V228
		G225	G229

Table 5

Sequence Identities Within the Kinase Domain and the Inhibitor-Binding Site for Human MEK1 Versus Other Members of the MEK Family						
Sequence Name (Human)	Kinase Domain Sequence Identity to MEK1		Ligand-Binding Site Sequence Identity (within 4 Å) to MEK1		Ligand-Binding Site Sequence Identity (within 5 Å) to MEK1	
	Counting gaps	Not counting gaps	Counting gaps	Not counting gaps	Counting gaps	Not counting gaps
MPK2	84.83	85.89	100	100	100	100
MPK3	35.26	41.88	71.43	71.43	62.96	62.96
MPK4	35.74	42.96	71.43	71.43	70.37	70.37
MPK5	38.11	46.82	80.95	80.95	81.48	81.48
MPK6	35.56	42.55	71.43	71.43	62.96	62.96
MPK7	34.45	40.79	61.90	61.90	62.96	62.96

Table 6

Sequence Identities Within the Kinase Domain and the ATP-Binding Site for Human MEK1 Versus Other Members of the MEK Family						
Sequence Name (Human)	Kinase Domain Sequence Identity to MEK1		ATP-Binding Site Sequence Identity (within 4 Å) to MEK1		ATP-Binding Site Sequence Identity (within 5 Å) to MEK1	
	Counting gaps	Not counting gaps	Counting gaps	Not counting gaps	Counting gaps	Not counting gaps
MPK2	84.83	85.89	100	100	100	100
MPK3	35.26	41.88	76.00	76.00	76.67	76.67
MPK4	35.74	42.96	68.00	68.00	66.67	66.67
MPK5	38.11	46.82	76.00	76.00	80.00	80.00
MPK6	35.56	42.55	76.00	76.00	76.67	76.67
MPK7	34.45	40.79	60.00	60.00	60.00	60.00

Table 7

A Detailed Description of the Secondary Structure of MEK1 as Determined by the X-ray Crystallographic Structural Analysis	
Secondary Structure	Amino Acid Residues
Unstructured*	62:67
Beta Sheet	68:76
Beta Sheet	81:87
Beta Sheet	92:98
Alpha Helix	105:120
Beta Sheet	129:134
Beta sheet	139:143
Beta Sheet	149:150
Alpha Helix	151:156
Alpha Helix	163:184
Beta Sheet	196:198
Beta Sheet	204:206
Alpha Helix	213:218
Flexible Loop*	219:231
Alpha Helix	232:236
Alpha Helix	243:258
Flexible Loop*	259:309
Alpha Helix	310:318
Alpha Helix	332:341
Alpha Helix	352:357
Alpha Helix	359:362
Alpha Helix	372:379
Unstructured*	380:383

* These features were not included in the structural model due to the lack of interpretable electron density.

Table 8

RMS Deviation Values for Selected C alpha and Backbone Atoms of MEK1 and MEK2 Structures*							
RMSD between overall MEK1 and MEK2 structures		RMSD between the kinase domain of MEK1 and MEK2 structures		RMSD between the 4 Å inhibitor binding site residues of MEK1 and MEK2		RMSD between the 5 Å inhibitor binding site residues of MEK1 and MEK2	
Using C alpha only	Using Backbone atoms	Using C alpha only	Using Backbone atoms	Using C alpha only	Using Backbone atoms	Using C alpha only	Using Backbone atoms
1.02	1.11	0.95	1.02	1.08	1.22	0.99	1.12

* The residues used in the RMS deviation calculations can be found in the embodiment.

SEQUENCE LISTING

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Claims

1. An isolated peptide selected from the group consisting of:

a Mitogen Activated Protein Kinase 1 /ERK kinase 1 (MEK1) peptide having an NH_2-terminal truncation lacking from at least 30 to at most 70 amino acid residues from the NH_2-terminal region of the full-length MEK1 peptide set forth in SEQ ID NO: 2, or a conservatively substituted variant thereof;
a MEK1 peptide having a deletion of insertion loop-forming amino acid residues selected from amino acid 280 to amino acid 323 of SEQ ID NO: 2 or at least 40 amino acids from between amino acid residue 264 and amino acid 310 of SEQ ID NO: 2, or a conservatively substituted variant thereof;
a peptide comprising (1) an NH_2-terminal truncation lacking from at least 30 to at most 70 amino acid residues from the NH_2-terminal region of the full-length MEK1 peptide set forth in SEQ ID NO: 2; and (2) a deletion of insertion loop-forming amino acid residues selected from amino acid 280 to amino acid 323 of SEQ ID NO: 2 or at least 40 amino acids from between amino acid residue 264 and amino acid 310 of SEQ ID NO: 2, or a conservatively substituted variant thereof;
a Mitogen Activated Protein Kinase 2/ERK kinase 2 (MEK2) peptide having an NH_2-terminal truncation lacking from at least 34 to at most 74 amino acid residues from the NH_2-terminal region of the full-length MEK2 peptide set forth in SEQ ID NO: 4, or a conservatively substituted variant thereof; and
a peptide that is defined by the structural coordinates of the MEK1 or MEK2 peptide as set forth in Table 1 or Table 2 or a related set of structural coordinates having a root mean square deviation of not more than about 1.25 Å away from the core C alpha atoms of the MEK1 or MEK2 structural coordinates as set forth in Table 1 or Table 2.

2. A peptide comprising a binding pocket selected from the group consisting of :

(a) a Mitogen Activated Protein Kinase 1 /ERK kinase 1 (MEK1) peptide ligand-binding pocket that is defined by the structural coordinates of the following amino acid residues within about 4 Å of a MEK1 inhibitor located in the ligand-binding site: G77, N78, G79, G80, K97, I99, L115, L118, V127, F129, I141, M143, C207, D208, F209, G210, V211, S212, L215, I216 and M219 of SEQ ID NO: 2, or a conservatively substituted variant thereof;
(b) a MEK1 peptide ligand-binding pocket that is defined by the structural coordinates of the following amino acid residues within about 5 Å of a MEK1 inhibitor located in the ligand-binding site: G77, N78, G79, G80, K97, 199, L115, L118, I126, V127, G128, F129, I141, M143, D190, N195, L206, C207, D208, F209, G210, V211, S212, L215, I216, M219 and F223 of SEQ ID NO: 2, or a conservatively substituted variant thereof;
(c) a Mitogen Activated Protein Kinase 2/ERK kinase 2 (MEK2) MEK2 peptide ligand-binding pocket that is defined by the structural coordinates of the following amino acid residues within about 4 Å of a MEK2 inhibitor located in the ligand-binding site: G81, N82, G83, G84, K101, I103, L119, L122, V131, F133, I145, M147, C211, D212, F213, G214, V215, S216, L219, I220, M223 of SEQ ID NO: 4, or a conservatively substituted variant thereof;
(d) a MEK2 peptide ligand-binding pocket that is defined by structural coordinates of the following amino acid residues within about 5 Å of a MEK2 inhibitor located in the ligand-binding site: G81, N82, G83, G84, K101, I103, L119, L122, I130, V131, G132, F133, I145, M147, D194, N199, L210, C211, D212, F213, G214, V215, S216, L219, I220, M223, F227.of SEQ ID NO: 4, or a conservatively substituted variant thereof;
(e) a MEK1 peptide cofactor-binding pocket that is defined by the structural coordinates of the following residues within about 4 Å of a cofactor located in the cofactor-binding site: L74, G75, A76, G77, N78, G80, V81,

V82, A95, K97, V127, M143, E144, H145, M146, G149, S150, D152, Q153, K192, S194, N195, L197, D208 and V224 of SEQ ID NO: 2, or a conservatively substituted variant thereof;
(f) a MEK1 peptide cofactor-binding pocket that is defined by the structural coordinates of the following residues within about 5 Å of a cofactor located in the cofactor-binding site: L74, G75, A76, G77, N78, G79, 80, V81, V82, A95, K97, V127, M143, E144, H145, M146, D147, G149, S150, D152, Q153, D190, K192, S194, N195, L197, C207, D208, V224 and G225 of SEQ ID NO:2, or a conservatively substituted variant thereof;
(g) a MEK2 peptide cofactor-binding pocket that is defined by the structural coordinates of the following residues within about 4 Å of a cofactor located in the cofactor-binding site: L78, G79, A80, G81, N82, G84, V85, V86, A99, K101, V131, M147, E148, H149, M150, G153, S154, D156, Q157, K196, S198, N199, L201, D212, V228 of SEQ ID NO: 4, or a conservatively substituted variant thereof;
(h) a MEK2 peptide cofactor-binding pocket that is defined by the structural coordinates of the following residues within about 5 Å of a cofactor in the cofactor-binding site: L78, G79, A80, G81, N82, G83, G84, V85, V86, A99, K101, V131, M147, E148, H149, M150, D151, G153, S154, D156, Q157, D194, K196, S198, N199, L201, C211, D212, V228, G229 of SEQ ID NO: 4, or a conservatively substituted variant thereof; and
(i) a binding pocket that is defined by the atoms found in the structural coordinates of the MEK1 or MEK2 peptide as set forth in Table 1 or Table 2, or in a related set of structural coordinates having a root mean square deviation of not more than about 1.25 Å away from the binding pocket C alpha atoms of the MEK1 or MEK2 binding pockets according to (a) - (h), or a conservatively substituted variant thereof.

3. A crystalline structure of a peptide:ligand:cofactor complex comprising a peptide according to claim 1 or claim 2.

4. Three-dimensional structural coordinates of a peptide:ligand:cofactor complex, comprising:

a peptide;
a cofactor; and
a ligand,

wherein the complex has the atomic coordinates set forth in Table 1 or Table 2, or a related set of structural coordinates having a root mean square deviation of not more than about 1.25 Å away from the core C alpha atoms of the MEK1 or MEK2 structural coordinates as set forth in Table 1 or Table 2.

5. An expression vector for producing the peptide according to claim 1 or claim 2 in a host cell comprising a polynucleotide encoding the modified peptide, and transcriptional and translational regulatory sequences functional in the host cell operably linked to the modified peptide.

6. A host cell stably transformed and transfected with a polynucleotide selected from the group consisting of a polynucleotide encoding the peptide according to claim 1 or claim 2, or a conservatively substituted variant thereof.

7. A method of utilizing molecular replacement to obtain structural information about a molecule or a molecular complex of unknown structure comprising:

crystallizing said molecule or molecular complex;
generating an X-ray diffraction pattern from said crystallized molecule or molecular complex; and
applying at least a portion of the structural coordinates set forth in Table 1 or Table 2, or a related set of structural coordinates having a root mean square deviation of not more than about 1.25 Å away from the core C alpha atoms of the MEK1 or MEK2 structural coordinates as set forth in Table 1 or Table 2, to the X-ray diffraction pattern to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown.

8. A method for generating a three-dimensional computer representation of a peptide according to claim 1 or claim 2, or a binding pocket thereof, comprising applying the atomic coordinates set forth in Table 1 or Table 2, or a related set of structural coordinates having a root mean square deviation of not more than about 1.25 Å away from the core C alpha atoms of the MEK1 or MEK2 structural coordinates as set forth in Table 1 or Table 2, to a computer algorithm to generate a three-dimensional representation of the peptide or peptide binding pocket.

9. A machine-readable medium having stored thereon data comprising the atomic coordinates as set forth in Table 1 or Table 2, or a related set of structural coordinates having a root mean square deviation of not more than about 1.25 Å away from the core C alpha atoms of the MEK1 or MEK2 structural coordinates as set forth in Table 1 or

Table 2.

10. A method for modifying or designing a chemical entity having the potential to associate with a peptide according to claim 1 or claim 2, comprising,

(a) generating a three-dimensional computer representation of the peptide or a binding pocket of the peptide; and
(b) generating a chemical entity that spatially conforms to the three-dimensional representation of the peptide or the peptide binding pocket, wherein the chemical entity is generated by a method comprising (i) assembling molecular fragments into the chemical entity; (ii) de novo design of the chemical entity or a fragment thereof; (iii) selecting the chemical entity from a small molecule database; or (iv) modifying a known inhibitor, or portion thereof, of MEK activity.

11. A method for screening and identifying a potential inhibitor or enhancer of the activity of a peptide according to claim 1 or claim 2, comprising:

(a) generating a three-dimensional computer representation of the peptide or a binding pocket of the peptide;
(b) applying an iterative process whereby a chemical entity is applied to the three-dimensional representation to determine whether the chemical entity associates with the peptide or peptide binding pocket; and
(c) evaluating the effect(s) of the chemical entity on peptide activity to determine whether the chemical entity functions as an activity inhibitor or enhancer.

12. A method for evaluating the potential of a chemical entity to associate with a peptide according to claim 1 or claim 2, comprising

(a) generating a three-dimensional representation of the peptide or a binding pocket of the peptide;
(b) applying a three-dimensional representation of a chemical entity to the three-dimensional representation; and
(c) quantifying the association between the chemical entity and the binding pocket.

13. The method according to any one of claims 8, 10, 11, or 12, wherein the peptide binding pocket is selected from the group consisting of:

(a) a Mitogen Activated Protein Kinase 1 /ERK kinase 1 (MEK1) peptide ligand-binding pocket that is defined by the structural coordinates of the following amino acid residues within about 4 Å of a MEK1 inhibitor located in the ligand-binding site: G77, N78, G79, G80, K97, I99, L115, L118, V127, F129, I141, M143, C207, D208, F209, G210, V211, S212, L215, I216 and M219 of SEQ ID NO: 2, or a conservatively substituted variant thereof;
(b) a MEK1 peptide ligand-binding pocket that is defined by the structural coordinates of the following amino acid residues within about 5 Å of a MEK1 inhibitor located in the ligand-binding site: G77, N78, G79, G80, K97, 199, L115, L118, I126, V127, G128, F129, I141, M143, D190, N195, L206, C207, D208, F209, G210, V211, S212, L215, I216, M219 and F223 of SEQ ID NO: 2, or a conservatively substituted variant thereof;
(c) a Mitogen Activated Protein Kinase 2/ERK kinase 2 (MEK2) MEK2 peptide ligand-binding pocket that is defined by the structural coordinates of the following amino acid residues within about 4 Å of a MEK2 inhibitor located in the ligand-binding site: G81, N82, G83, G84, K101, I103, L119, L122, V131, F133, I145, M147, C211, D212, F213, G214, V215, S216, L219, I220, M223 of SEQ ID NO: 4, or a conservatively substituted variant thereof;
(d) a MEK2 peptide ligand-binding pocket that is defined by structural coordinates of the following amino acid residues within about 5 Å of a MEK2 inhibitor located in the ligand-binding site: G81, N82, G83, G84, K101, I103, L119, L122, I130, V131, G132, F133, I145, M147, D194, N199, L210, C211, D212, F213, G214, V215, S216, L219, I220, M223, F227 of SEQ ID NO: 4, or a conservatively substituted variant thereof;
(e) a MEK1 peptide cofactor-binding pocket that is defined by the structural coordinates of the following residues within about 4 Å of a cofactor located in the cofactor-binding site: L74, G75, A76, G77, N78, G80, V81, V82, A95, K97, V127, M143, E144, H145, M146, G149, S150, D152, Q153, K192, S194, N195, L197, D208 and V224 of SEQ ID NO: 2, or a conservatively substituted variant thereof;
(f) a MEK1 peptide cofactor-binding pocket that is defined by the structural coordinates of the following residues within about 5 Å of a cofactor in the cofactor-binding site: L74, G75, A76, G77, N78, G79, 80, V81, V82, A95, K97, V127, M143, E144, H145, M146, D147, G149, S150, D152, Q153, D190, K192, S194, N195, L197, C207, D208, V224 and G225 of SEQ ID NO:2, or a conservatively substituted variant thereof;

(g) a MEK2 peptide cofactor-binding pocket that is defined by the structural coordinates of the following residues within about 4 Å of a cofactor located in the cofactor-binding site: L78, G79, A80, G81, N82, G84, V85, V86, A99, K101, V131, M147, E148, H149, M150, G153, S154, D156, Q157, K196, S198, N199, L201, D212, V228 of SEQ ID NO: 4, or a conservatively substituted variant thereof;
(h) a MEK2 peptide cofactor-binding pocket that is defined by the structural coordinates of the following residues within about 5 Å of a cofactor located in the cofactor-binding site: L78, G79, A80, G81, N82, G83, G84, V85, V86, A99, K101, V131, M147, E148, H149, M150, D151, G153, S154, D156, Q157, D194, K196, S198, N199, L201, C211, D212, V228, G229 of SEQ ID NO: 4, or a conservatively substituted variant thereof; and
(i) a binding pocket that is defined by the atoms found in the structural coordinates of the MEK1 or MEK2 peptide as set forth in Table 1 or Table 2, or in a related set of structural coordinates having a root mean square deviation of not more than about 1.25 Å away from the binding pocket C alpha atoms of the MEK1 or MEK2 binding pockets according to (a) - (h), or a conservatively substituted variant thereof.

14. A method of purifying a peptide according to claim 1 or claim 2 from a fermentation broth containing the peptide and contaminant proteins other than the peptide, comprising subjecting the fermentation broth to immobilized metal chelate chromatography comprising pyrrole-2-carboxylate, zinc chloride, and an immobilized metal selected from the group consisting of nickel, zinc, copper and cobalt.

15. A method of growing the crystalline structure according to claim 3, comprising:

providing a peptide solution comprising the peptide, a ligand, a cofactor, a buffering agent, a reducing agent, and a source of ionic strength;
providing a precipitant solution comprising

(a) if the peptide is MEK1 peptide, polyethylene glycol (PEG), a source of ionic strength, a buffering agent, and a reducing agent; or
(b) if the peptide is MEK2 peptide, a source of ionic strength, a buffering agent, and a reducing agent;

mixing a droplet of said peptide solution with a droplet of said precipitant solution;
suspending the resulting mixed droplet over a well of said precipitant solution at a vapor pressure of the solution in said well being lower than in the resulting solution in the mixed droplet; and
allowing the suspended mixed droplet to stand for a prolonged period until a peptide:ligand:cofactor ternary complex crystal grows to a size suitable for X-ray diffraction.

FIG. 1

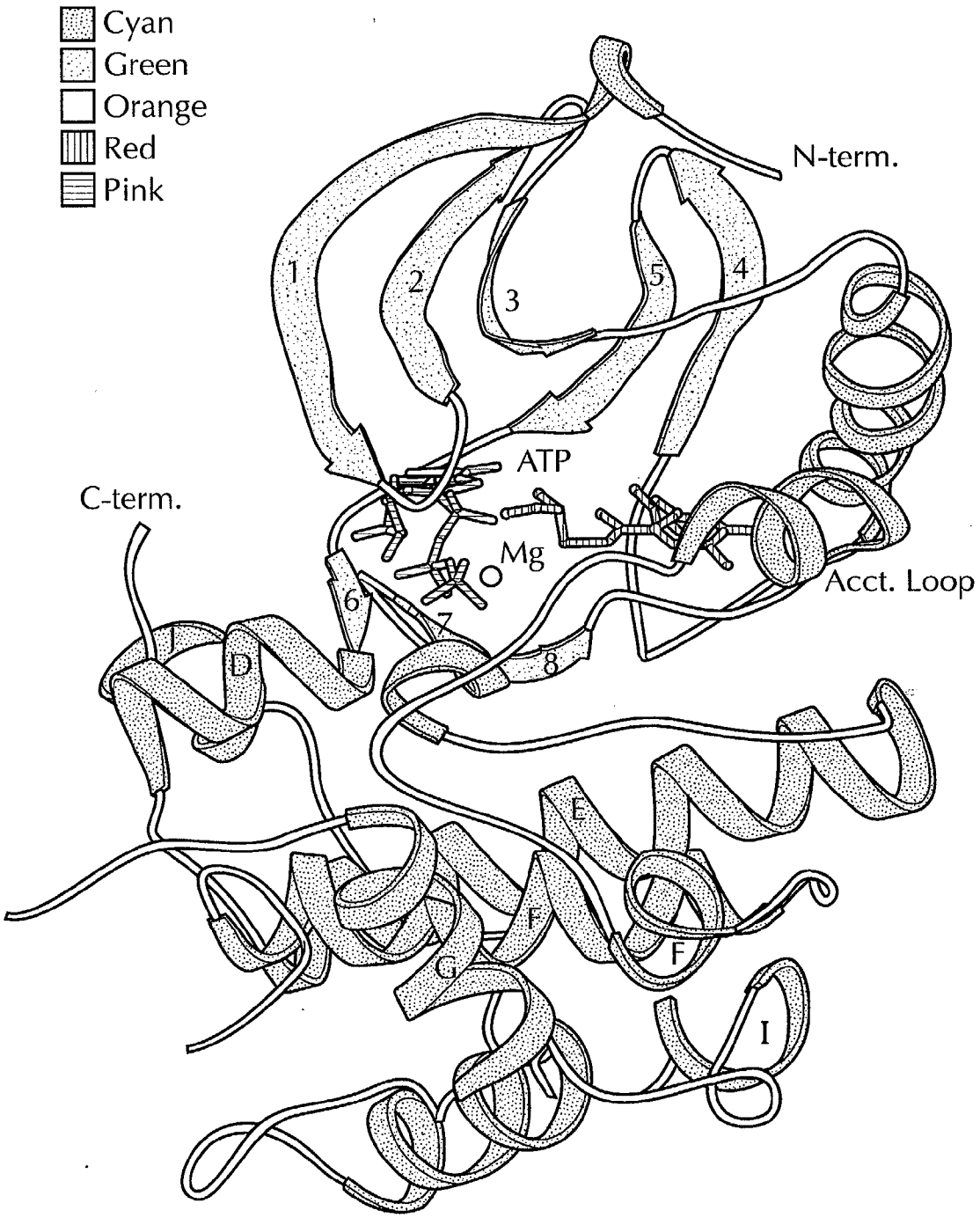
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FIG. 2

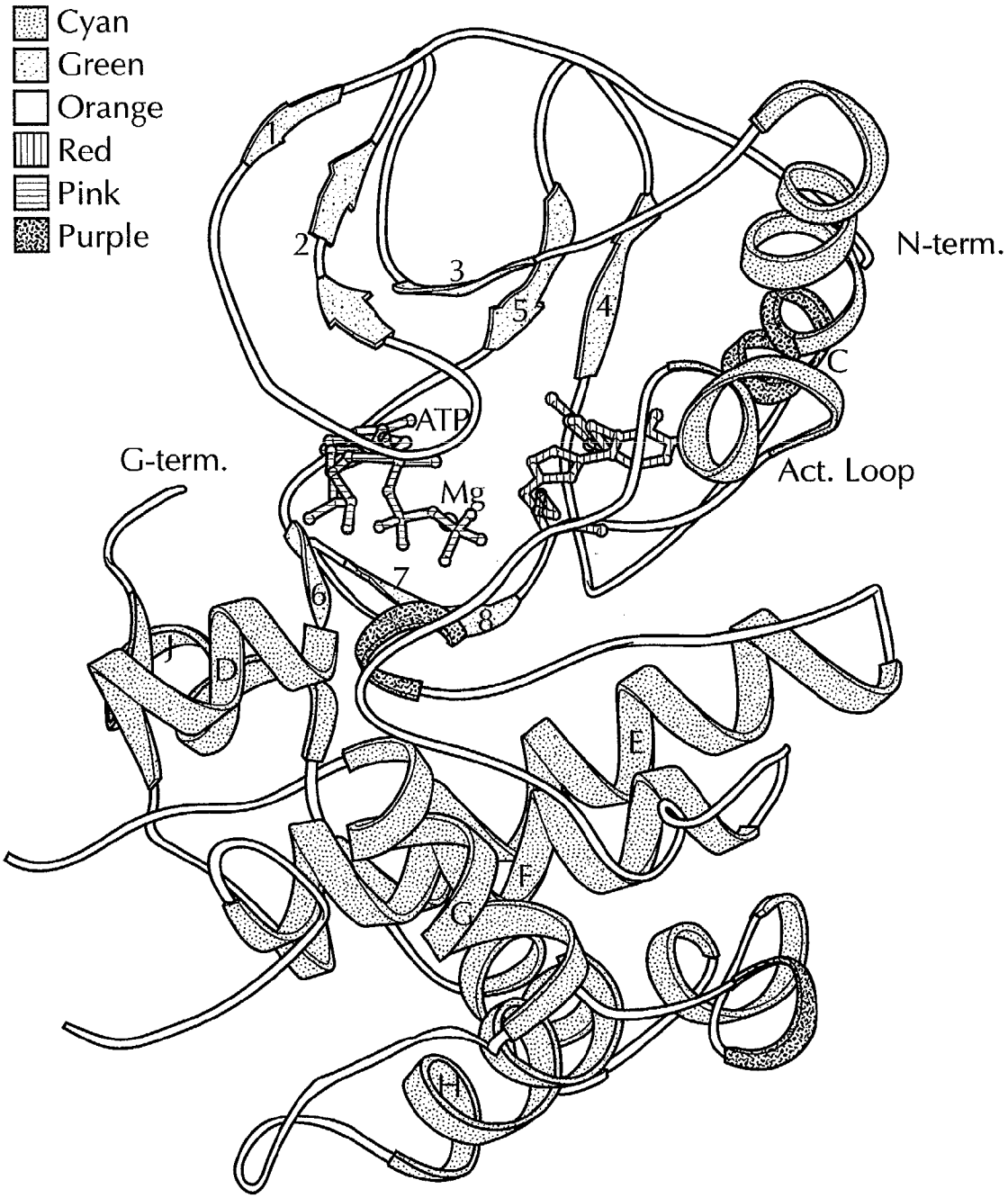
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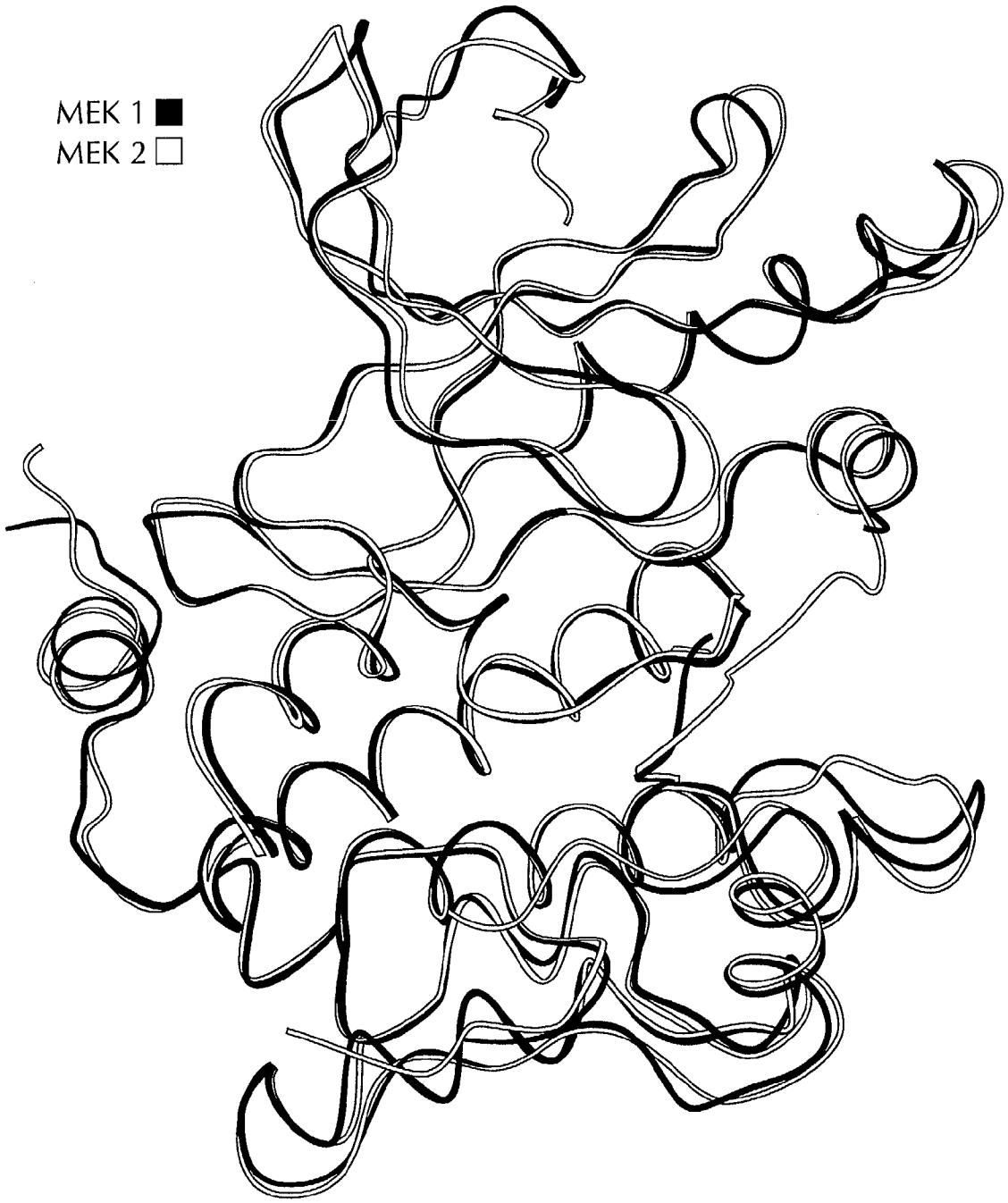
FIG. 3



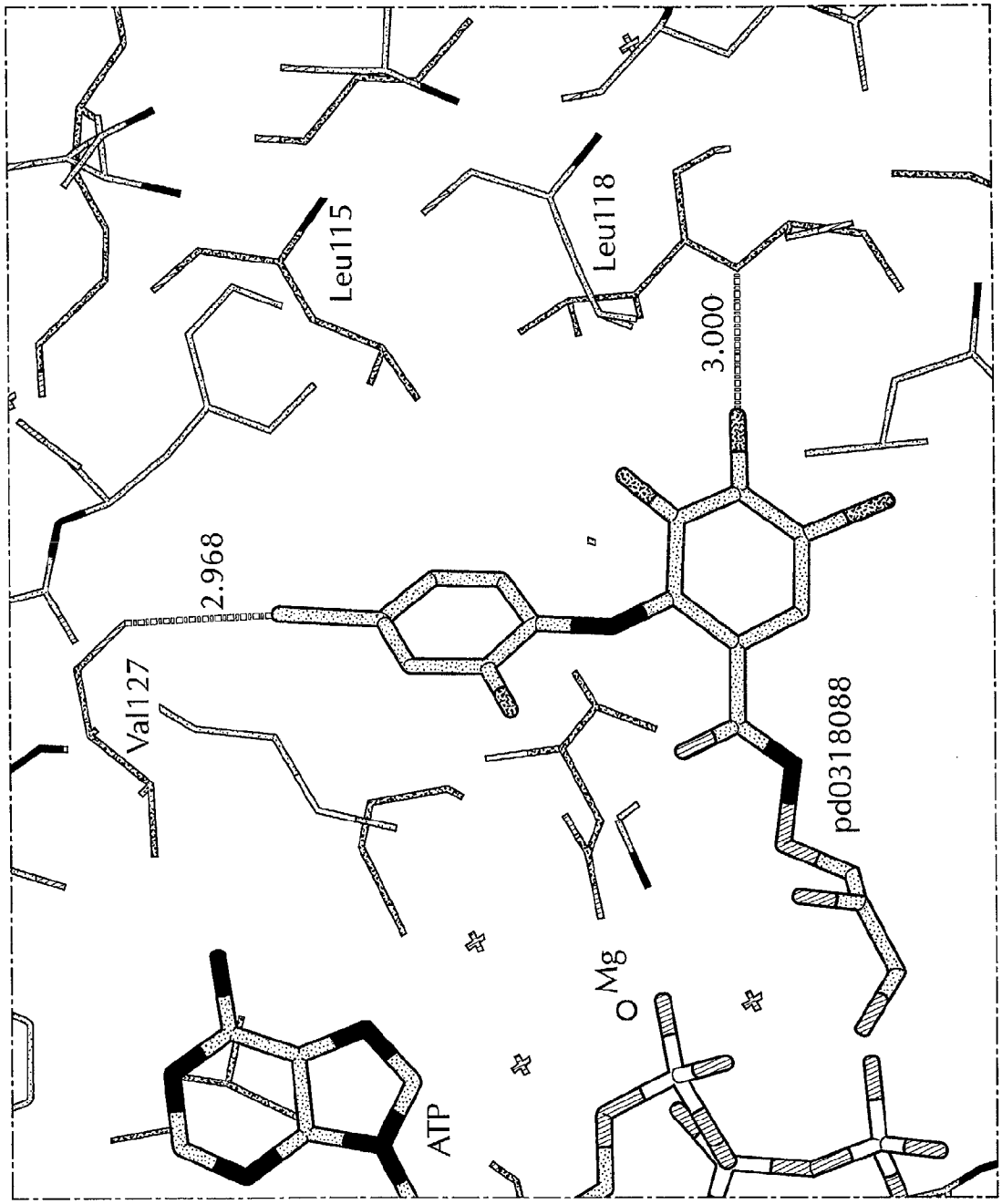


FIG. 4

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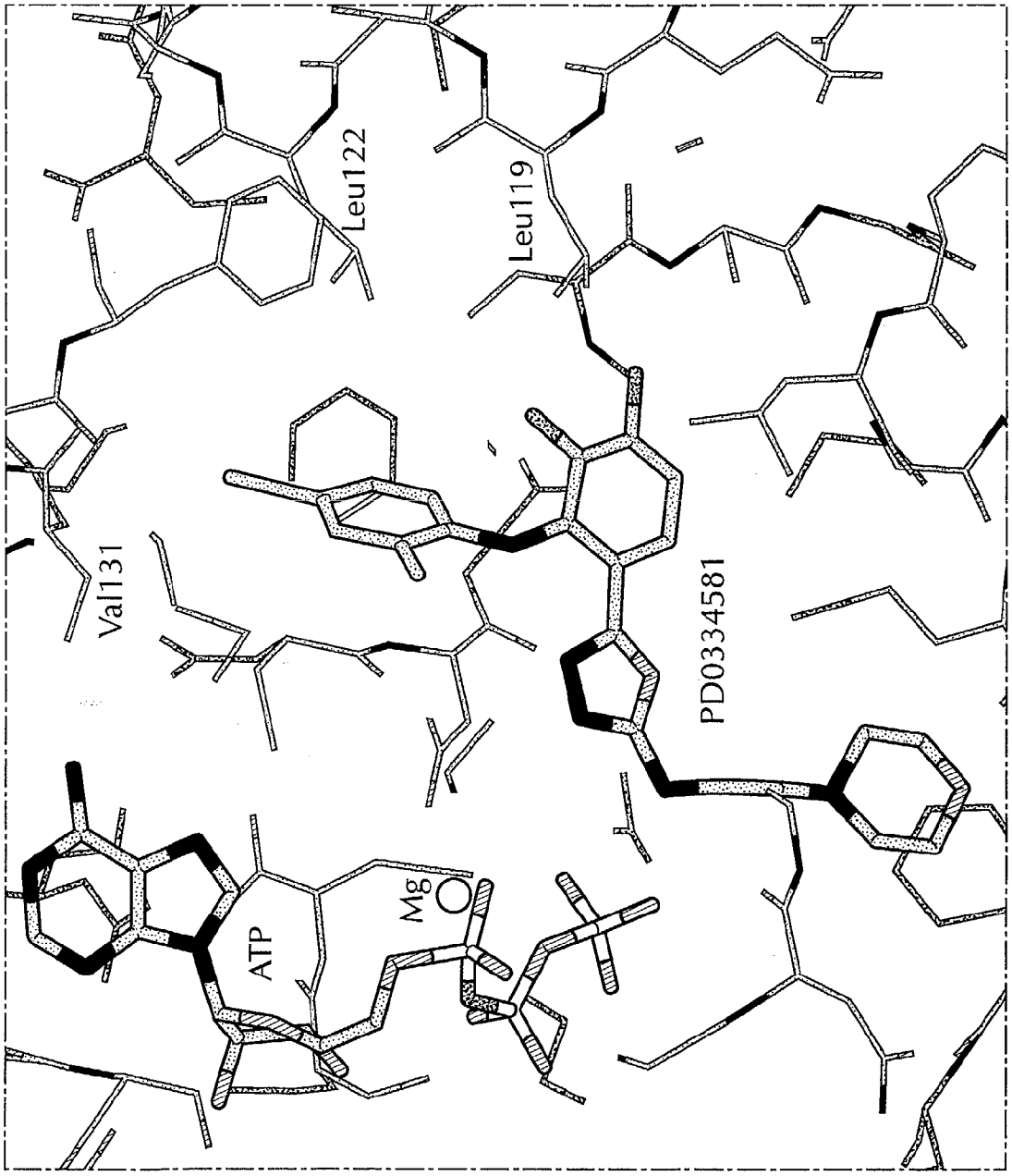

FIG. 5

Cyan
Dark green
green
Red
Yellow

European Patent Office

PARTIAL EUROPEAN SEARCH REPORT

which under Rule 45 of the European Patent Convention shall be considered, for the purposes of subsequent proceedings, as the European search report

Application Number EP 02 25 8507

DOCUMENTS CONSIDERED TO BE RELEVANT

Category	Citation of document with indication, where appropriate, of relevant passages	Relevant to claim	CLASSIFICATION OF THE APPLICATION (Int.Cl.7)
X	DUESBERY ET AL: "Proteolytic inactivation of MAP-kinase-kinase by anthrax lethal factor" SCIENCE, AMERICAN ASSOCIATION FOR THE ADVANCEMENT OF SCIENCE,, US, vol. 280, no. 5364, 1 May 1998 (1998-05-01), pages 734-737, XP002115820 ISSN: 0036-8075 * page 736, column 2, line 16 - line 22; figure 3C * ---	1,2,5,6, 14	C12N9/12
X	MANSOUR SAM J ET AL: "Interdependent domains controlling the enzymatic activity of mitogen-activated protein kinase kinase 1." BIOCHEMISTRY, vol. 35, no. 48, 1996, pages 15529-15536, XP002235966 ISSN: 0006-2960 * page 15531, column 2, line 16 * --- -/--	1,2,5,6, 14	TECHNICAL FIELDS SEARCHED (Int.Cl.7) C12N

INCOMPLETE SEARCH

The Search Division considers that the present application, or one or more of its claims, does/do not comply with the EPC to such an extent that a meaningful search into the state of the art cannot be carried out, or can only be carried out partially, for these claims.

Claims searched completely :

Claims searched incompletely :

Claims not searched :

Reason for the limitation of the search:

see sheet C

Place of search	Date of completion of the search	Examiner
MUNICH	26 March 2003	Petri, B

CATEGORY OF CITED DOCUMENTS

X : particularly relevant if taken alone
Y : particularly relevant if combined with another document of the same category
A : technological background
O : non-written disclosure
P : intermediate document

T : theory or principle underlying the invention
E : earlier patent document, but published on, or after the filing date
D : document cited in the application
L : document cited for other reasons

& : member of the same patent family, corresponding document

EPO FORM 1503 03.82 (P04C07)

European Patent Office

INCOMPLETE SEARCH SHEET C

Application Number
EP 02 25 8507

Claim(s) searched incompletely:
13

Claim(s) not searched:
4, 7-9, 11-12

Reason for the limitation of the search (non-patentable invention(s)):

The claims 4, 7-9, 11-12, and 13 as far it refers back to claims 8, 11-12 relate to subject-matter excluded from patentability under Article 52 (2)(d). Given that the claims are formulated in terms of such subject-matter or merely specify features which relate to presentation of information, the above mentioned claims will not be searched.

The claims 7-8, 11-12 and 13 as far it refers back to claims 8, 11-12, relate to subject-matter excluded from patentability under Article 52 (2)(c) EPC. Given that the claims are formulated in terms of such subject-matter or merely specify features which relate to programs for computers, the above mentioned claims will not be searched.

European Patent Office

PARTIAL EUROPEAN SEARCH REPORT

Application Number
EP 02 25 8507

DOCUMENTS CONSIDERED TO BE RELEVANT			CLASSIFICATION OF THE APPLICATION (Int.Cl.7)
Category	Citation of document with indication, where appropriate, of relevant passages	Relevant to claim	
X	DATABASE SWALL [Online] 1 July 1993 (1993-07-01) "MPK1_Human; MEK1" retrieved from EBI Database accession no. Q02750 XP002235970 * the whole document * ---	2,5,6,14	
X	DATABASE SWALL [Online] 1 June 1994 (1994-06-01) "MPK2_Human; MEK2" retrieved from EBI Database accession no. P36507 XP002235971 * the whole document * ---	2,5,6,14	TECHNICAL FIELDS SEARCHED (Int.Cl.7)
A	WANG ZHULUN ET AL: "The structure of mitogen-activated protein kinase p38 at 2.1-A resolution." PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES, vol. 94, no. 6, 1997, pages 2327-2332, XP002235967 1997 ISSN: 0027-8424 * the whole document * ---	3,15	
A	LEI MING ET AL: "Structure of PAK1 in an autoinhibited conformation reveals a multistage activation switch." CELL, vol. 102, no. 3, 4 August 2000 (2000-08-04), pages 387-397, XP002235968 ISSN: 0092-8674 * the whole document * --- -/--	3,15	

EPO FORM 1503 03.82 (P04C10)

European Patent Office

PARTIAL EUROPEAN SEARCH REPORT

Application Number
EP 02 25 8507

DOCUMENTS CONSIDERED TO BE RELEVANT			CLASSIFICATION OF THE APPLICATION (Int.Cl.7)
Category	Citation of document with indication, where appropriate, of relevant passages	Relevant to claim	
A	PEARSON GRAY ET AL: "Mitogen-activated protein (MAP) kinase pathways: Regulation and physiological functions." ENDOCRINE REVIEWS, vol. 22, no. 2, April 2001 (2001-04), pages 153-183, XP002235969 ISSN: 0163-769X ---		
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